



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:47 AM UTC

PDB ID : 3RED / pdb_00003red
Title : 3.0 Å structure of the Prunus mume hydroxynitrile lyase isozyme-1
Authors : Cielo, C.B.C.; Yamane, T.; Asano, Y.; Watanabe, N.; Suzuki, A.; Fukuta, Y.
Deposited on : 2011-04-04
Resolution : 3.03 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

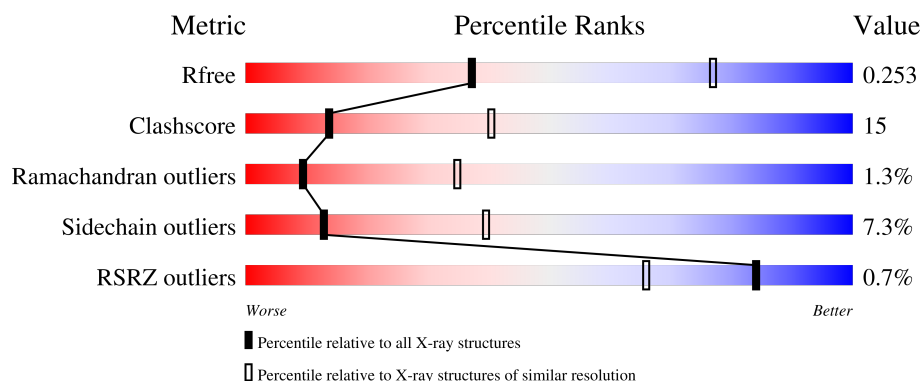
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	521	68% 29% ..
1	B	521	69% 26% ..
1	C	521	74% 22% ..
1	D	521	64% 30% ..
1	E	521	71% 25% ..

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Mol	Chain	Length	Quality of chain
1	F	521	% 67% 30%
1	G	521	67% 28%
1	H	521	% 67% 28% 5%
1	I	521	% 69% 26%
1	J	521	% 69% 27%
1	K	521	% 68% 28%
1	L	521	61% 35%

2 Entry composition

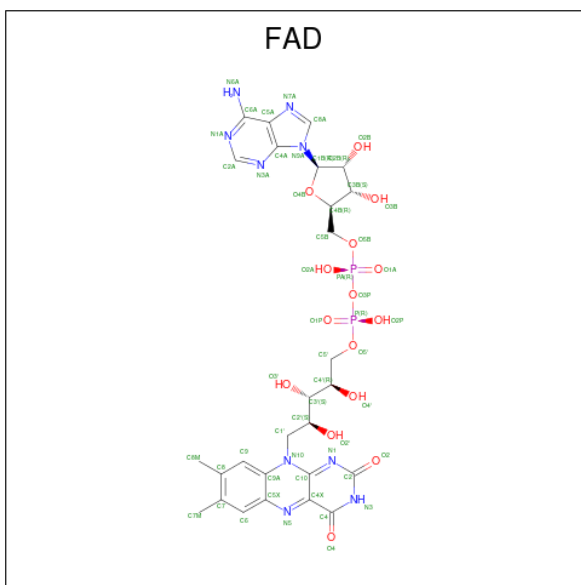
There are 2 unique types of molecules in this entry. The entry contains 48604 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	2	0
			4001	2547	657	788	9			
1	B	521	Total	C	N	O	S	0	2	0
			3999	2547	659	784	9			
1	C	521	Total	C	N	O	S	0	1	0
			3993	2543	656	785	9			
1	D	521	Total	C	N	O	S	0	1	0
			3993	2543	656	785	9			
1	E	521	Total	C	N	O	S	0	1	0
			3993	2543	656	785	9			
1	F	521	Total	C	N	O	S	0	2	0
			4001	2548	659	785	9			
1	G	521	Total	C	N	O	S	0	2	0
			4001	2548	659	785	9			
1	H	521	Total	C	N	O	S	0	2	0
			4001	2548	659	785	9			
1	I	521	Total	C	N	O	S	0	1	0
			3993	2543	656	785	9			
1	J	521	Total	C	N	O	S	0	1	0
			3991	2543	656	783	9			
1	K	521	Total	C	N	O	S	0	2	0
			4001	2548	659	785	9			
1	L	521	Total	C	N	O	S	0	2	0
			4001	2548	659	785	9			

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

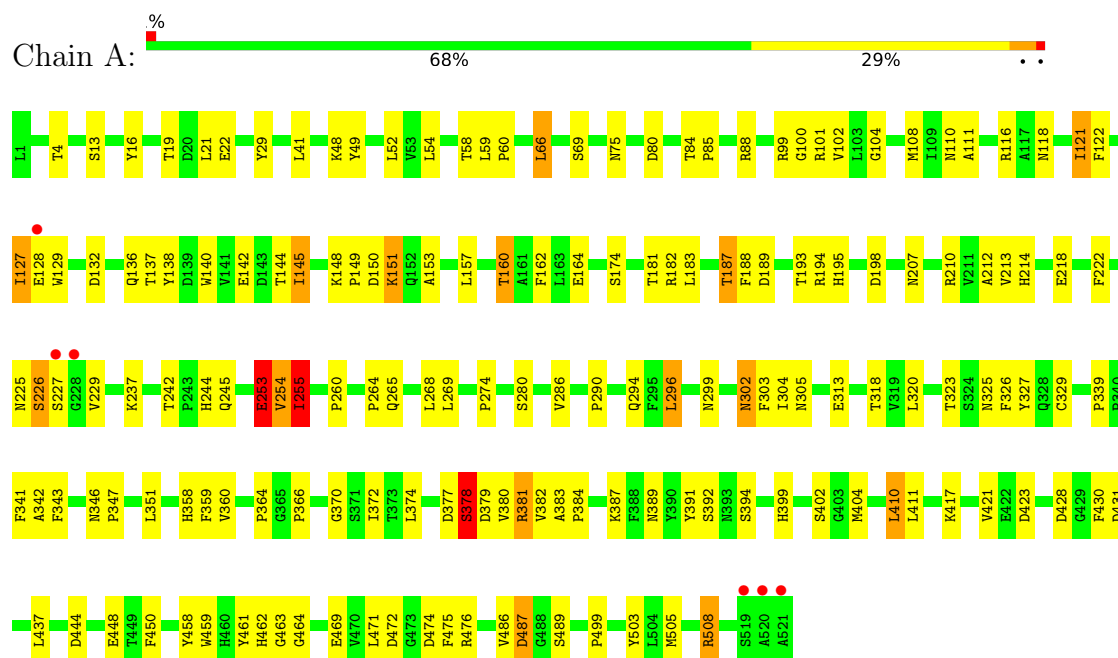


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	G	1	Total 53	C 27	N 9	O 15	P 2	0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

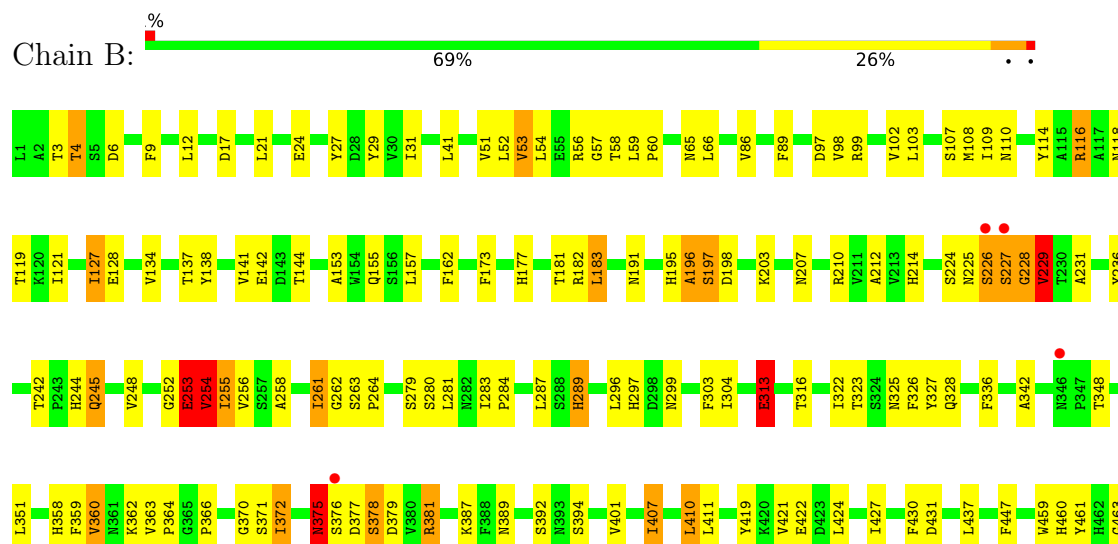
3 Residue-property plots

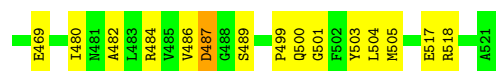
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

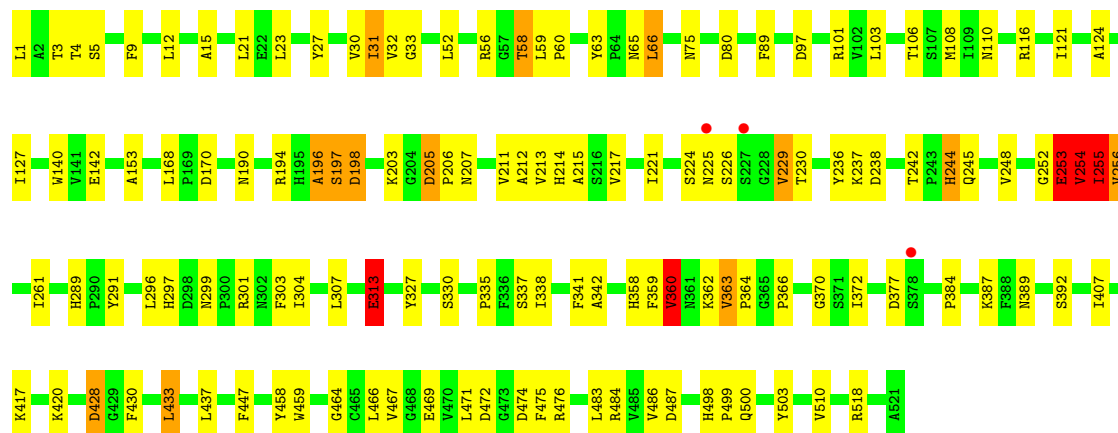
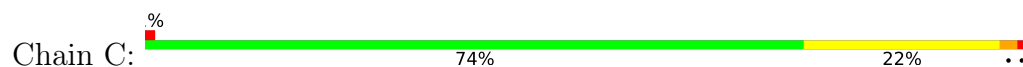


• Molecule 1: Hydroxynitrile lyase

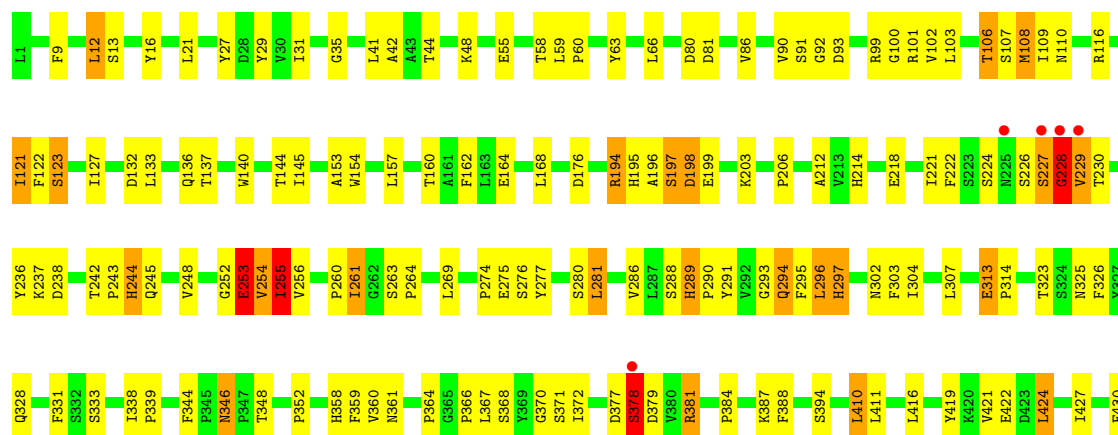




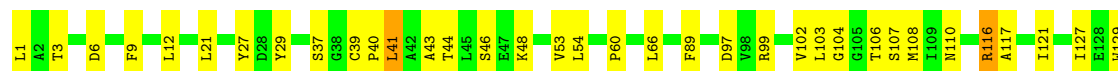
• Molecule 1: Hydroxynitrile lyase

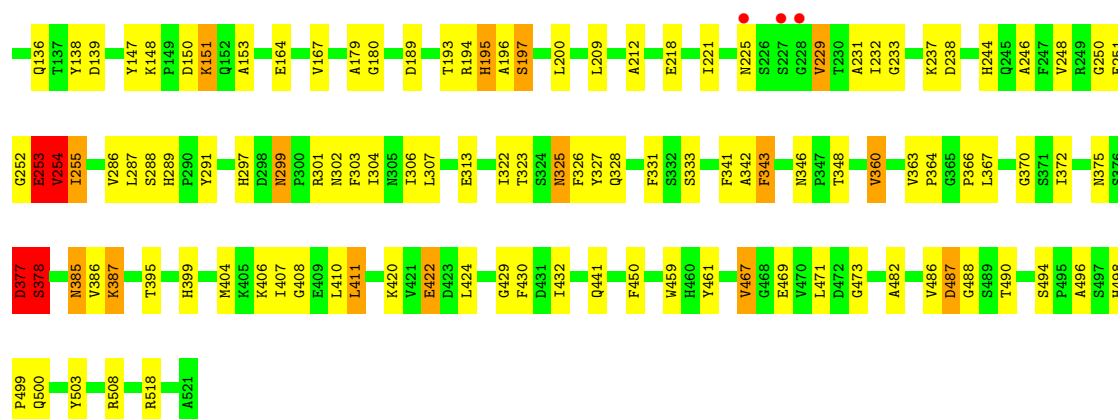


• Molecule 1: Hydroxynitrile lyase

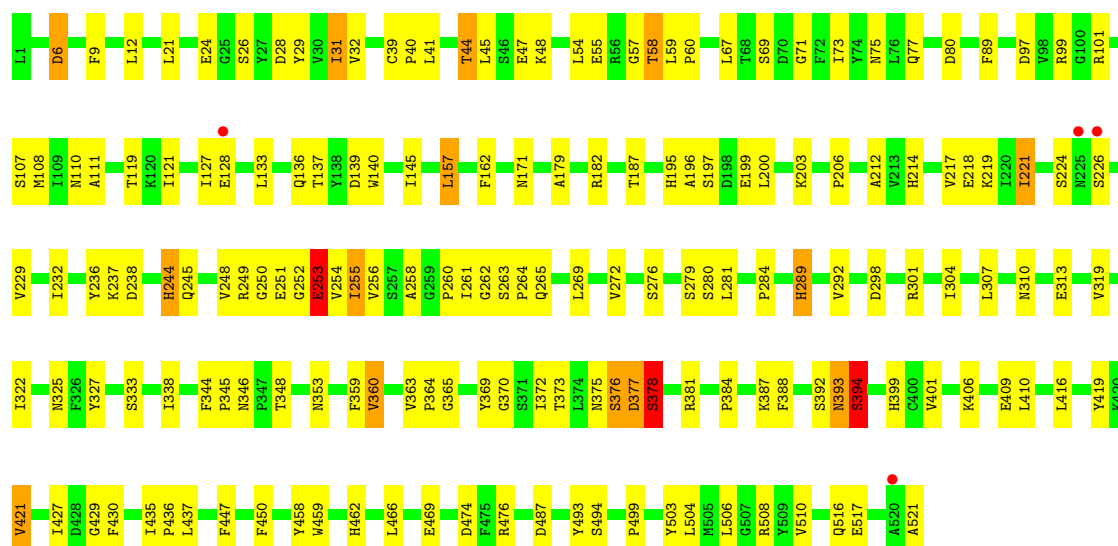


• Molecule 1: Hydroxynitrile lyase

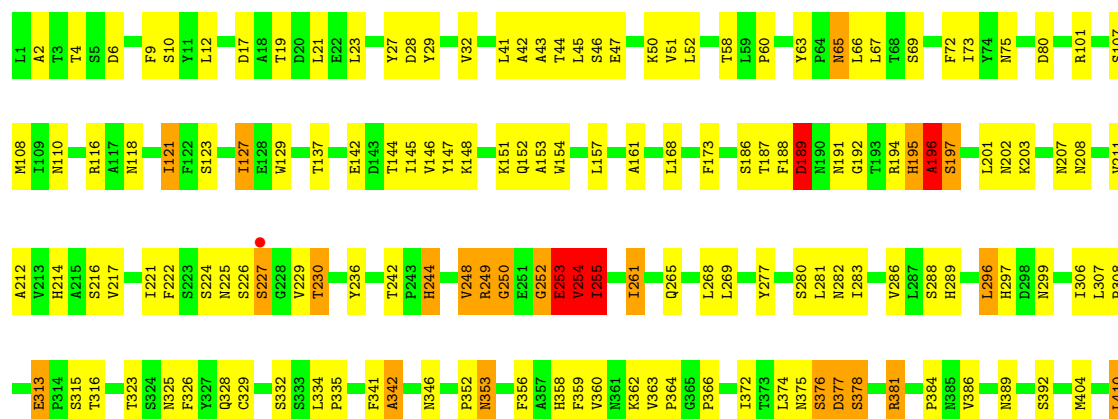




• Molecule 1: Hydroxynitrile lyase

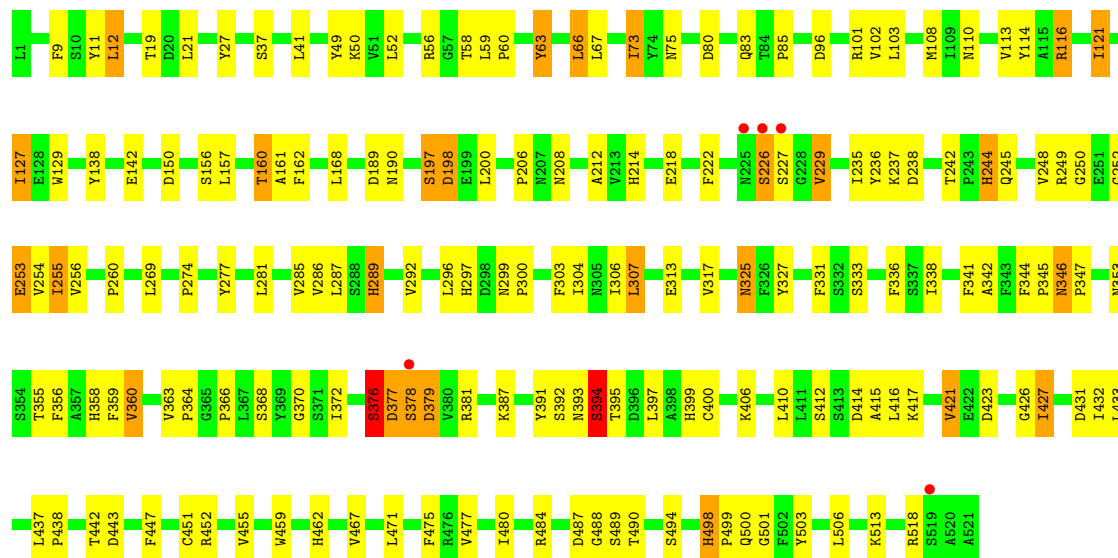


• Molecule 1: Hydroxynitrile lyase

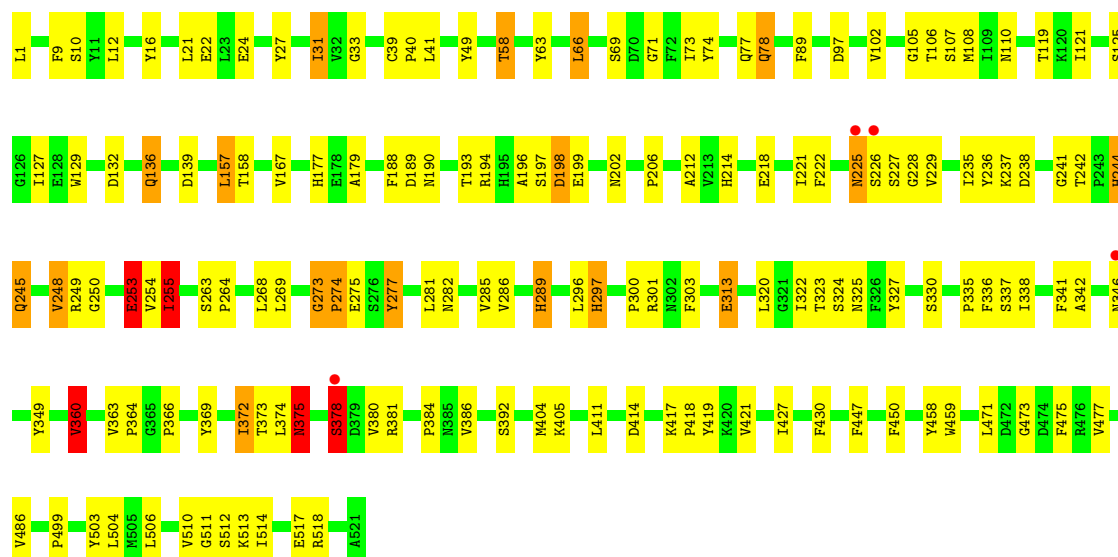




• Molecule 1: Hydroxynitrile lyase

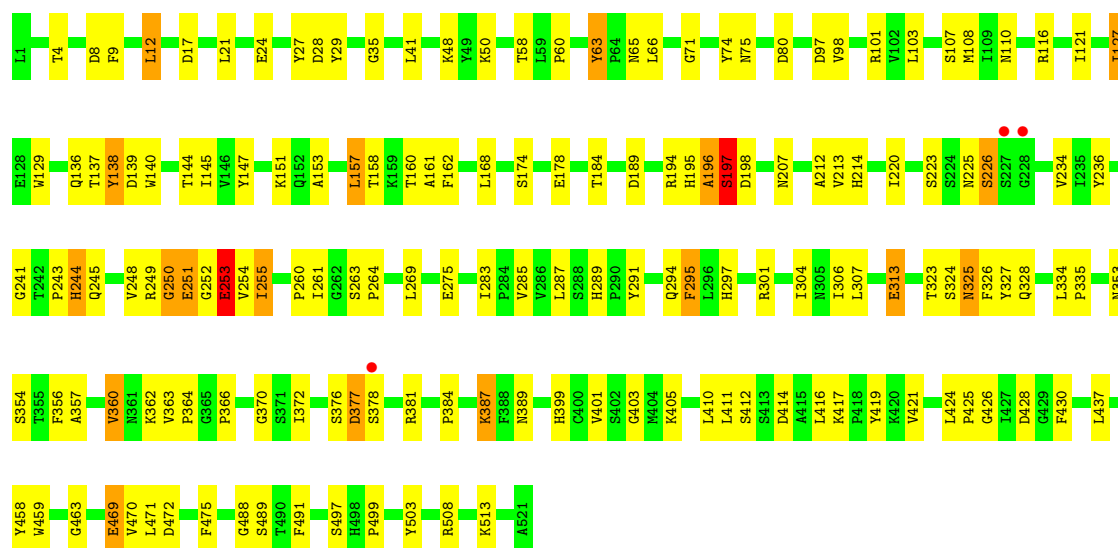


• Molecule 1: Hydroxynitrile lyase

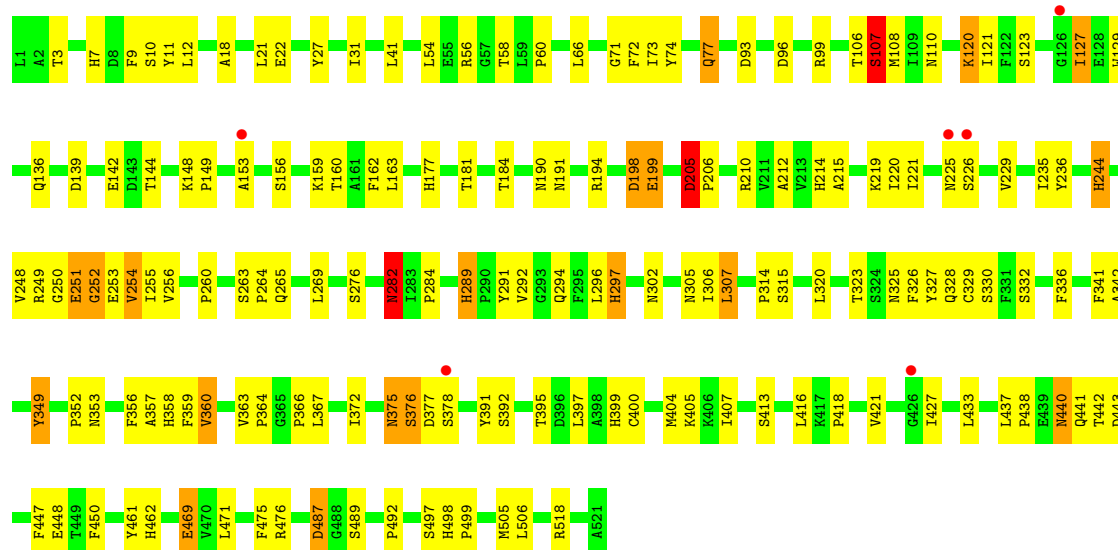


• Molecule 1: Hydroxynitrile lyase

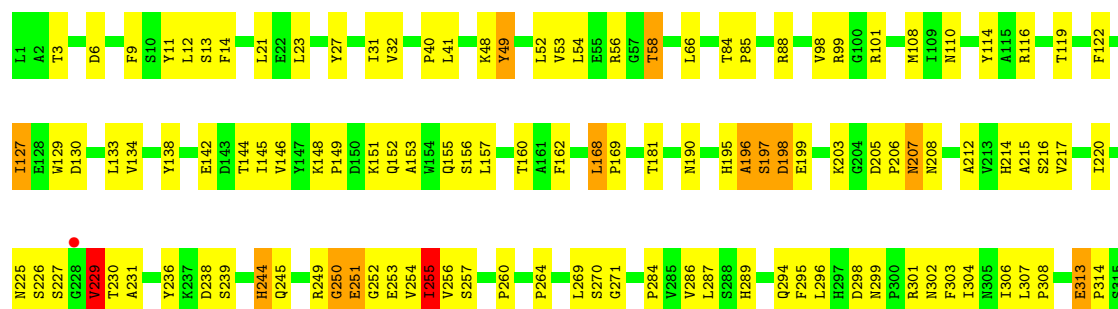


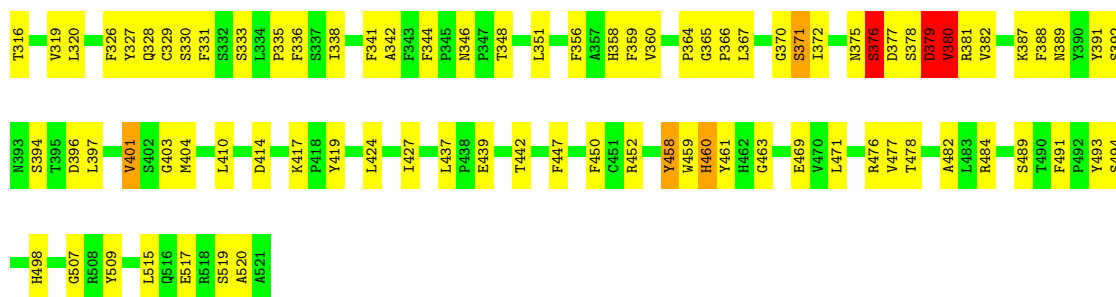


• Molecule 1: Hydroxynitrile lyase



• Molecule 1: Hydroxynitrile lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.02Å 113.30Å 169.49Å 89.92° 79.13° 80.83°	Depositor
Resolution (Å)	10.97 – 3.03 10.97 – 3.03	Depositor EDS
% Data completeness (in resolution range)	96.0 (10.97-3.03) 94.1 (10.97-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.253 0.195 , 0.253	Depositor DCC
R_{free} test set	7404 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48604	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.91	13/4106 (0.3%)	1.07	16/5606 (0.3%)
1	B	0.88	9/4107 (0.2%)	1.10	20/5606 (0.4%)
1	C	0.87	6/4098 (0.1%)	1.08	19/5595 (0.3%)
1	D	1.01	16/4098 (0.4%)	1.15	26/5595 (0.5%)
1	E	0.90	12/4098 (0.3%)	1.09	24/5595 (0.4%)
1	F	0.91	7/4109 (0.2%)	1.10	19/5609 (0.3%)
1	G	0.95	13/4109 (0.3%)	1.10	20/5609 (0.4%)
1	H	0.94	13/4109 (0.3%)	1.11	24/5609 (0.4%)
1	I	0.91	10/4098 (0.2%)	1.08	18/5595 (0.3%)
1	J	0.89	8/4096 (0.2%)	1.06	17/5593 (0.3%)
1	K	0.93	11/4109 (0.3%)	1.07	12/5609 (0.2%)
1	L	0.95	12/4109 (0.3%)	1.07	21/5609 (0.4%)
All	All	0.92	130/49246 (0.3%)	1.09	236/67230 (0.4%)

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	B	0	2
1	C	0	2
1	D	0	3
1	E	0	1
1	F	0	2
1	G	0	2
1	I	0	2
All	All	0	14

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	195	HIS	CA-C	-11.57	1.38	1.52
1	L	380	VAL	N-CA	-7.35	1.38	1.46
1	H	255	ILE	C-O	-7.21	1.16	1.24
1	L	254	VAL	CA-CB	-7.07	1.45	1.54
1	G	195	HIS	C-O	-6.98	1.15	1.23
1	L	255	ILE	C-O	-6.86	1.17	1.24
1	A	255	ILE	C-O	-6.86	1.17	1.24
1	A	254	VAL	C-O	-6.81	1.16	1.24
1	I	255	ILE	CA-CB	-6.75	1.46	1.54
1	K	254	VAL	C-O	-6.71	1.16	1.24
1	E	195	HIS	C-O	-6.62	1.16	1.23
1	D	195	HIS	N-CA	-6.57	1.38	1.46
1	A	255	ILE	CA-C	-6.33	1.45	1.52
1	H	325	ASN	CG-OD1	6.21	1.35	1.23
1	E	196	ALA	CA-CB	-6.19	1.44	1.53
1	B	252	GLY	N-CA	6.17	1.49	1.44
1	E	255	ILE	C-O	-6.17	1.17	1.24
1	D	196	ALA	CA-CB	-6.16	1.44	1.53
1	G	196	ALA	CA-CB	-6.11	1.43	1.53
1	C	253	GLU	C-O	-6.07	1.16	1.23
1	K	375	ASN	CG-OD1	6.06	1.35	1.23
1	H	83	GLN	CD-OE1	6.04	1.35	1.23
1	L	207	ASN	CG-OD1	6.02	1.34	1.23
1	K	190	ASN	CG-OD1	5.96	1.34	1.23
1	L	245	GLN	CD-OE1	5.96	1.34	1.23
1	B	254	VAL	C-O	-5.95	1.17	1.24
1	E	225	ASN	CG-OD1	5.95	1.34	1.23
1	L	255	ILE	CA-C	-5.92	1.45	1.52
1	B	256	VAL	C-O	-5.90	1.17	1.24
1	I	375	ASN	CG-OD1	5.88	1.34	1.23
1	J	254	VAL	CA-CB	-5.85	1.47	1.54
1	H	245	GLN	CD-OE1	5.83	1.34	1.23
1	K	191	ASN	CG-OD1	5.81	1.34	1.23
1	D	256	VAL	C-O	-5.79	1.17	1.24
1	I	78	GLN	CD-OE1	5.79	1.34	1.23
1	L	190	ASN	CG-OD1	5.79	1.34	1.23
1	A	225	ASN	CG-ND2	-5.79	1.21	1.33
1	G	481	ASN	CG-OD1	5.74	1.34	1.23
1	K	225	ASN	CG-OD1	5.74	1.34	1.23
1	D	441	GLN	CD-OE1	5.71	1.34	1.23
1	D	245	GLN	CD-OE1	5.70	1.34	1.23
1	L	380	VAL	CA-CB	-5.70	1.48	1.54
1	J	255	ILE	C-O	-5.67	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	375	ASN	CG-OD1	5.67	1.34	1.23
1	B	256	VAL	CA-CB	-5.66	1.47	1.54
1	G	225	ASN	CG-OD1	5.66	1.34	1.23
1	I	190	ASN	CG-OD1	5.65	1.34	1.23
1	L	254	VAL	N-CA	-5.64	1.39	1.46
1	H	297	HIS	ND1-CE1	5.62	1.38	1.32
1	L	328	GLN	CD-OE1	5.60	1.34	1.23
1	C	245	GLN	CD-OE1	5.58	1.34	1.23
1	D	297	HIS	ND1-CE1	5.58	1.38	1.32
1	F	399	HIS	ND1-CE1	5.56	1.38	1.32
1	E	385	ASN	CG-OD1	5.56	1.34	1.23
1	F	244	HIS	ND1-CE1	5.54	1.38	1.32
1	H	190	ASN	CG-OD1	5.52	1.34	1.23
1	F	255	ILE	C-O	-5.52	1.18	1.24
1	B	289	HIS	ND1-CE1	5.52	1.38	1.32
1	G	254	VAL	C-O	-5.49	1.17	1.24
1	E	244	HIS	ND1-CE1	5.47	1.38	1.32
1	H	253	GLU	N-CA	-5.47	1.39	1.46
1	F	75	ASN	CG-OD1	5.47	1.33	1.23
1	I	244	HIS	ND1-CE1	5.46	1.38	1.32
1	H	399	HIS	ND1-CE1	5.46	1.38	1.32
1	L	460	HIS	ND1-CE1	5.46	1.38	1.32
1	C	244	HIS	ND1-CE1	5.45	1.38	1.32
1	G	252	GLY	N-CA	5.44	1.50	1.44
1	E	399	HIS	ND1-CE1	5.43	1.38	1.32
1	G	244	HIS	ND1-CE1	5.43	1.38	1.32
1	A	244	HIS	ND1-CE1	5.43	1.38	1.32
1	K	244	HIS	ND1-CE1	5.43	1.38	1.32
1	K	282	ASN	CG-OD1	5.42	1.33	1.23
1	A	214	HIS	ND1-CE1	5.40	1.38	1.32
1	H	376	SER	CA-C	-5.40	1.46	1.52
1	B	255	ILE	C-O	-5.40	1.18	1.24
1	F	256	VAL	CA-CB	-5.39	1.47	1.54
1	J	245	GLN	CD-OE1	5.38	1.33	1.23
1	D	361	ASN	CG-OD1	5.38	1.33	1.23
1	A	399	HIS	ND1-CE1	5.38	1.38	1.32
1	K	252	GLY	C-O	-5.37	1.18	1.23
1	B	155	GLN	CD-OE1	5.36	1.33	1.23
1	F	245	GLN	CD-OE1	5.33	1.33	1.23
1	I	245	GLN	CD-OE1	5.33	1.33	1.23
1	B	245	GLN	CD-OE1	5.32	1.33	1.23
1	H	244	HIS	ND1-CE1	5.32	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	136	GLN	CD-NE2	-5.31	1.22	1.33
1	L	256	VAL	C-O	-5.30	1.18	1.24
1	D	244	HIS	ND1-CE1	5.30	1.37	1.32
1	K	297	HIS	ND1-CE1	5.30	1.37	1.32
1	E	302	ASN	CG-OD1	5.28	1.33	1.23
1	A	265	GLN	CD-NE2	-5.27	1.22	1.33
1	E	196	ALA	N-CA	-5.25	1.38	1.46
1	G	187	THR	C-O	-5.25	1.17	1.24
1	J	244	HIS	ND1-CE1	5.25	1.37	1.32
1	I	177	HIS	ND1-CE1	5.25	1.37	1.32
1	D	302	ASN	CG-OD1	5.24	1.33	1.23
1	J	399	HIS	ND1-CE1	5.24	1.37	1.32
1	G	375	ASN	CG-OD1	5.23	1.33	1.23
1	I	297	HIS	ND1-CE1	5.23	1.37	1.32
1	K	77	GLN	CD-OE1	5.23	1.33	1.23
1	H	256	VAL	C-O	-5.22	1.18	1.24
1	C	190	ASN	CG-OD1	5.19	1.33	1.23
1	D	294	GLN	CD-OE1	5.19	1.33	1.23
1	B	191	ASN	CG-OD1	5.19	1.33	1.23
1	A	75	ASN	CG-OD1	5.18	1.33	1.23
1	J	253	GLU	CA-C	-5.18	1.46	1.52
1	I	289	HIS	ND1-CE1	5.18	1.37	1.32
1	C	190	ASN	CG-ND2	-5.17	1.22	1.33
1	E	375	ASN	CG-ND2	-5.17	1.22	1.33
1	D	255	ILE	C-O	-5.16	1.18	1.24
1	D	255	ILE	N-CA	-5.16	1.40	1.46
1	D	108	MET	CA-C	-5.16	1.45	1.52
1	G	328	GLN	CD-OE1	5.14	1.33	1.23
1	G	75	ASN	CG-OD1	5.13	1.33	1.23
1	E	325	ASN	CG-OD1	5.13	1.33	1.23
1	D	136	GLN	CD-OE1	5.11	1.33	1.23
1	K	107	SER	C-O	-5.09	1.17	1.24
1	C	75	ASN	CG-OD1	5.08	1.33	1.23
1	G	191	ASN	C-O	-5.08	1.17	1.24
1	A	214	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	253	GLU	C-O	-5.06	1.17	1.23
1	A	302	ASN	CG-OD1	5.05	1.33	1.23
1	J	75	ASN	CG-OD1	5.04	1.33	1.23
1	H	75	ASN	CG-OD1	5.04	1.33	1.23
1	E	375	ASN	CG-OD1	5.04	1.33	1.23
1	A	245	GLN	CD-OE1	5.03	1.33	1.23
1	H	254	VAL	CA-CB	-5.03	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	297	HIS	CD2-NE2	-5.02	1.32	1.37
1	J	283	ILE	CA-CB	5.01	1.58	1.54
1	G	255	ILE	C-O	-5.00	1.18	1.24

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	HIS	N-CA-C	-13.90	86.24	108.90
1	L	255	ILE	N-CA-C	-8.82	95.32	108.46
1	L	254	VAL	N-CA-C	-8.76	95.56	108.87
1	J	307	LEU	CA-C-N	8.37	125.77	119.66
1	J	307	LEU	C-N-CA	8.37	125.77	119.66
1	H	338	ILE	N-CA-C	-8.33	102.36	109.19
1	G	498	HIS	CA-C-N	8.30	129.33	120.12
1	G	498	HIS	C-N-CA	8.30	129.33	120.12
1	C	205	ASP	CA-C-N	8.29	127.95	119.82
1	C	205	ASP	C-N-CA	8.29	127.95	119.82
1	L	380	VAL	N-CA-C	-8.28	102.62	112.98
1	H	255	ILE	N-CA-C	-8.13	95.61	108.86
1	C	254	VAL	N-CA-C	-7.85	97.08	109.17
1	G	253	GLU	CA-C-N	7.70	135.82	121.97
1	G	253	GLU	C-N-CA	7.70	135.82	121.97
1	L	344	PHE	CA-C-N	7.63	129.38	119.84
1	L	344	PHE	C-N-CA	7.63	129.38	119.84
1	I	273	GLY	CA-C-N	7.54	129.27	119.84
1	I	273	GLY	C-N-CA	7.54	129.27	119.84
1	F	255	ILE	N-CA-C	-7.54	97.61	108.17
1	C	313	GLU	CA-C-N	7.48	127.76	119.90
1	C	313	GLU	C-N-CA	7.48	127.76	119.90
1	C	198	ASP	N-CA-C	-7.46	104.33	113.50
1	G	191	ASN	N-CA-C	-7.42	104.07	113.72
1	B	253	GLU	CA-C-N	7.30	135.12	121.97
1	B	253	GLU	C-N-CA	7.30	135.12	121.97
1	D	198	ASP	N-CA-C	-7.28	104.55	113.50
1	D	253	GLU	CA-C-N	7.11	134.49	121.70
1	D	253	GLU	C-N-CA	7.11	134.49	121.70
1	H	377	ASP	N-CA-C	7.01	121.09	112.54
1	G	283	ILE	CA-C-N	-7.01	112.42	119.99
1	G	283	ILE	C-N-CA	-7.01	112.42	119.99
1	G	346	ASN	N-CA-C	7.01	114.53	108.22
1	J	196	ALA	CA-C-N	6.87	134.06	121.70
1	J	196	ALA	C-N-CA	6.87	134.06	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	325	ASN	N-CA-C	6.87	121.36	112.92
1	E	253	GLU	CA-C-N	6.80	134.21	121.97
1	E	253	GLU	C-N-CA	6.80	134.21	121.97
1	F	399	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	F	394	SER	CA-C-N	6.72	130.20	120.38
1	F	394	SER	C-N-CA	6.72	130.20	120.38
1	F	253	GLU	CA-C-N	6.71	133.78	121.70
1	F	253	GLU	C-N-CA	6.71	133.78	121.70
1	H	346	ASN	N-CA-C	6.71	115.86	108.14
1	D	196	ALA	N-CA-C	6.71	118.31	108.86
1	H	379	ASP	N-CA-C	-6.70	98.71	109.96
1	A	399	HIS	CB-CG-CD2	-6.69	122.50	131.20
1	F	253	GLU	N-CA-C	-6.68	96.56	110.80
1	H	399	HIS	CB-CG-CD2	-6.68	122.52	131.20
1	H	297	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	A	225	ASN	N-CA-C	6.65	119.52	109.41
1	K	349	TYR	CA-C-N	6.64	127.00	119.83
1	K	349	TYR	C-N-CA	6.64	127.00	119.83
1	I	177	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	A	214	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	B	289	HIS	CB-CG-CD2	-6.61	122.60	131.20
1	J	138	TYR	N-CA-C	-6.59	104.02	111.07
1	E	399	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	K	297	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	D	255	ILE	N-CA-C	-6.54	99.07	108.48
1	G	244	HIS	CB-CG-CD2	-6.53	122.72	131.20
1	J	399	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	B	360	VAL	N-CA-C	6.49	119.44	108.86
1	B	196	ALA	CA-C-N	6.48	133.36	121.70
1	B	196	ALA	C-N-CA	6.48	133.36	121.70
1	L	460	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	L	196	ALA	N-CA-C	-6.47	102.45	110.41
1	B	254	VAL	N-CA-C	6.47	122.79	109.34
1	A	253	GLU	N-CA-C	6.46	118.59	108.96
1	H	244	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	I	289	HIS	CB-CG-CD2	-6.42	122.86	131.20
1	J	244	HIS	CB-CG-CD2	-6.42	122.86	131.20
1	J	63	TYR	CA-C-N	6.42	126.34	119.28
1	J	63	TYR	C-N-CA	6.42	126.34	119.28
1	C	244	HIS	CB-CG-CD2	-6.41	122.86	131.20
1	F	244	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	L	491	PHE	CA-C-N	6.39	125.82	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	491	PHE	C-N-CA	6.39	125.82	118.85
1	G	189	ASP	N-CA-C	6.39	119.91	110.46
1	D	297	HIS	CB-CG-CD2	-6.38	122.90	131.20
1	E	244	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	F	360	VAL	CB-CA-C	-6.34	102.13	111.19
1	C	254	VAL	CA-C-N	6.34	133.11	121.70
1	C	254	VAL	C-N-CA	6.34	133.11	121.70
1	I	297	HIS	CB-CG-CD2	-6.32	122.98	131.20
1	D	255	ILE	CB-CA-C	6.31	120.03	110.62
1	D	244	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	K	244	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	E	255	ILE	N-CA-C	-6.22	99.52	108.48
1	E	253	GLU	N-CA-C	-6.21	97.57	110.80
1	I	244	HIS	CB-CG-CD2	-6.21	123.12	131.20
1	G	187	THR	N-CA-C	-6.20	105.57	112.57
1	E	363	VAL	CA-C-N	6.16	126.13	119.78
1	E	363	VAL	C-N-CA	6.16	126.13	119.78
1	H	307	LEU	CA-C-N	6.14	124.08	119.66
1	H	307	LEU	C-N-CA	6.14	124.08	119.66
1	A	244	HIS	CB-CG-CD2	-6.13	123.22	131.20
1	D	424	LEU	CA-C-N	-6.07	114.30	120.85
1	D	424	LEU	C-N-CA	-6.07	114.30	120.85
1	B	198	ASP	N-CA-C	-6.05	105.72	113.23
1	G	196	ALA	N-CA-C	-6.04	97.94	110.80
1	H	63	TYR	CA-C-N	6.04	126.47	119.47
1	H	63	TYR	C-N-CA	6.04	126.47	119.47
1	C	196	ALA	CA-C-N	6.04	132.57	121.70
1	C	196	ALA	C-N-CA	6.04	132.57	121.70
1	L	371	SER	N-CA-C	5.98	118.95	109.50
1	D	468	GLY	N-CA-C	-5.97	107.08	115.32
1	F	399	HIS	CB-CG-ND1	5.92	131.59	122.70
1	A	104	GLY	N-CA-C	-5.92	107.23	114.92
1	D	108	MET	N-CA-C	-5.91	105.26	112.88
1	H	254	VAL	N-CA-C	-5.87	99.94	108.87
1	H	399	HIS	CB-CG-ND1	5.85	131.47	122.70
1	I	253	GLU	CA-C-N	5.85	132.23	121.70
1	I	253	GLU	C-N-CA	5.85	132.23	121.70
1	G	196	ALA	CA-C-N	5.84	132.21	121.70
1	G	196	ALA	C-N-CA	5.84	132.21	121.70
1	L	49	TYR	N-CA-C	5.83	118.42	109.38
1	A	399	HIS	CB-CG-ND1	5.82	131.44	122.70
1	K	205	ASP	CA-C-N	5.80	127.09	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	205	ASP	C-N-CA	5.80	127.09	119.84
1	I	198	ASP	N-CA-C	-5.78	105.33	112.90
1	B	289	HIS	CB-CG-ND1	5.78	131.37	122.70
1	E	498	HIS	CA-C-N	5.77	125.39	119.56
1	E	498	HIS	C-N-CA	5.77	125.39	119.56
1	E	399	HIS	CB-CG-ND1	5.76	131.35	122.70
1	A	148	LYS	CA-C-N	5.76	125.67	119.85
1	A	148	LYS	C-N-CA	5.76	125.67	119.85
1	B	313	GLU	CA-C-N	5.76	126.09	119.93
1	B	313	GLU	C-N-CA	5.76	126.09	119.93
1	I	49	TYR	N-CA-C	5.73	118.72	110.30
1	I	297	HIS	CB-CG-ND1	5.72	131.28	122.70
1	G	308	PRO	O-C-N	5.72	123.94	121.31
1	H	297	HIS	CB-CG-ND1	5.71	131.26	122.70
1	J	399	HIS	CB-CG-ND1	5.71	131.26	122.70
1	K	297	HIS	CB-CG-ND1	5.69	131.23	122.70
1	I	228	GLY	N-CA-C	-5.68	105.27	112.54
1	K	391	TYR	N-CA-C	5.68	120.02	113.38
1	A	100	GLY	N-CA-C	5.65	118.43	111.93
1	I	177	HIS	CB-CG-ND1	5.65	131.18	122.70
1	L	460	HIS	CB-CG-ND1	5.65	131.17	122.70
1	D	297	HIS	CB-CG-ND1	5.63	131.14	122.70
1	A	214	HIS	CB-CG-ND1	5.61	131.12	122.70
1	E	441	GLN	N-CA-C	5.60	119.38	112.54
1	F	378	SER	CA-C-N	-5.59	112.94	121.66
1	F	378	SER	C-N-CA	-5.59	112.94	121.66
1	E	343	PHE	N-CA-C	-5.58	105.11	111.14
1	C	196	ALA	N-CA-C	-5.58	103.12	110.43
1	B	375	ASN	CA-C-N	5.57	131.73	121.70
1	B	375	ASN	C-N-CA	5.57	131.73	121.70
1	D	289	HIS	CA-C-N	5.55	125.39	119.28
1	D	289	HIS	C-N-CA	5.55	125.39	119.28
1	F	333	SER	N-CA-C	5.53	117.48	109.07
1	H	244	HIS	CB-CG-ND1	5.52	130.98	122.70
1	F	244	HIS	CB-CG-ND1	5.52	130.98	122.70
1	D	344	PHE	CA-C-N	5.51	125.03	119.19
1	D	344	PHE	C-N-CA	5.51	125.03	119.19
1	G	244	HIS	CB-CG-ND1	5.50	130.96	122.70
1	I	244	HIS	CB-CG-ND1	5.50	130.96	122.70
1	D	244	HIS	CB-CG-ND1	5.50	130.94	122.70
1	C	363	VAL	CA-C-N	5.48	125.47	120.21
1	C	363	VAL	C-N-CA	5.48	125.47	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	360	VAL	N-CA-C	5.48	117.80	108.86
1	D	195	HIS	CA-C-O	5.48	126.28	120.36
1	E	377	ASP	CA-C-N	5.46	131.54	121.70
1	E	377	ASP	C-N-CA	5.46	131.54	121.70
1	K	31	ILE	CB-CA-C	-5.46	103.49	110.98
1	C	466	LEU	N-CA-C	5.46	119.14	109.96
1	F	466	LEU	N-CA-C	5.46	118.36	110.28
1	C	229	VAL	N-CA-C	5.46	116.05	108.84
1	G	255	ILE	N-CA-C	-5.46	100.47	108.11
1	C	244	HIS	CB-CG-ND1	5.45	130.88	122.70
1	J	244	HIS	CB-CG-ND1	5.45	130.88	122.70
1	B	17	ASP	N-CA-C	-5.44	102.34	110.23
1	F	369	TYR	N-CA-C	5.44	116.90	109.18
1	D	228	GLY	N-CA-C	-5.43	100.32	113.18
1	E	244	HIS	CB-CG-ND1	5.42	130.84	122.70
1	K	244	HIS	CB-CG-ND1	5.42	130.84	122.70
1	E	299	ASN	CA-C-N	5.36	125.12	119.76
1	E	299	ASN	C-N-CA	5.36	125.12	119.76
1	J	356	PHE	N-CA-C	5.36	117.34	109.24
1	H	73	ILE	CB-CA-C	-5.36	105.02	111.88
1	G	313	GLU	N-CA-C	5.35	116.39	109.65
1	E	432	ILE	N-CA-C	5.33	115.77	107.99
1	L	196	ALA	CA-C-N	5.33	131.29	121.70
1	L	196	ALA	C-N-CA	5.33	131.29	121.70
1	B	363	VAL	CA-C-N	5.31	125.21	119.85
1	B	363	VAL	C-N-CA	5.31	125.21	119.85
1	I	289	HIS	CB-CG-ND1	5.31	130.66	122.70
1	E	494	SER	CA-C-N	5.30	125.77	120.04
1	E	494	SER	C-N-CA	5.30	125.77	120.04
1	E	307	LEU	CA-C-N	5.30	125.84	120.38
1	E	307	LEU	C-N-CA	5.30	125.84	120.38
1	A	145	ILE	N-CA-C	5.29	117.49	111.88
1	J	491	PHE	CA-C-N	5.28	124.60	118.85
1	J	491	PHE	C-N-CA	5.28	124.60	118.85
1	D	378	SER	CA-C-N	-5.27	113.63	122.17
1	D	378	SER	C-N-CA	-5.27	113.63	122.17
1	H	198	ASP	N-CA-C	-5.26	106.00	112.90
1	J	470	VAL	CB-CA-C	-5.26	106.25	111.30
1	A	244	HIS	CB-CG-ND1	5.26	130.59	122.70
1	H	494	SER	CA-C-N	5.25	124.94	119.64
1	H	494	SER	C-N-CA	5.25	124.94	119.64
1	L	379	ASP	N-CA-C	-5.25	99.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	198	ASP	N-CA-C	-5.25	105.62	112.23
1	A	19	THR	N-CA-C	-5.24	106.39	112.89
1	C	229	VAL	CB-CA-C	-5.22	104.33	111.33
1	K	220	ILE	CB-CA-C	-5.21	104.65	110.96
1	F	307	LEU	CA-C-N	5.21	123.46	119.66
1	F	307	LEU	C-N-CA	5.21	123.46	119.66
1	I	360	VAL	N-CA-C	5.17	117.49	108.95
1	I	125	SER	N-CA-C	5.17	116.60	111.07
1	B	375	ASN	N-CA-C	5.17	121.81	110.80
1	C	360	VAL	N-CA-C	5.17	115.92	108.48
1	L	333	SER	N-CA-C	5.17	117.10	108.99
1	A	417	LYS	CA-C-N	-5.16	114.72	120.45
1	A	417	LYS	C-N-CA	-5.16	114.72	120.45
1	D	455	VAL	N-CA-C	5.15	116.65	109.80
1	H	455	VAL	N-CA-C	5.14	116.21	109.58
1	D	421	VAL	N-CA-C	-5.13	106.14	111.58
1	D	176	ASP	N-CA-C	5.10	117.92	109.46
1	H	150	ASP	N-CA-C	5.10	117.11	110.43
1	B	191	ASN	N-CA-C	-5.10	107.11	113.38
1	B	242	THR	CA-C-N	5.07	126.18	119.84
1	B	242	THR	C-N-CA	5.07	126.18	119.84
1	L	498	HIS	CA-C-N	5.07	126.08	120.45
1	L	498	HIS	C-N-CA	5.07	126.08	120.45
1	L	328	GLN	N-CA-C	5.06	116.88	109.24
1	F	28	ASP	N-CA-C	-5.05	105.43	112.45
1	I	225	ASN	N-CA-C	5.05	116.40	107.61
1	G	253	GLU	N-CA-C	-5.03	100.09	110.80
1	G	254	VAL	N-CA-C	5.03	119.79	109.34
1	L	229	VAL	N-CA-C	-5.02	103.02	109.30
1	H	498	HIS	CA-C-N	5.02	124.63	119.56
1	H	498	HIS	C-N-CA	5.02	124.63	119.56
1	E	254	VAL	N-CA-C	5.02	119.78	109.34
1	J	254	VAL	N-CA-C	-5.02	101.19	108.36

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	253	GLU	Peptide,Mainchain
1	C	253	GLU	Peptide
1	C	254	VAL	Peptide
1	D	194	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	D	253	GLU	Peptide,Mainchain
1	E	253	GLU	Peptide
1	F	253	GLU	Peptide,Mainchain
1	G	253	GLU	Peptide,Mainchain
1	I	253	GLU	Peptide,Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4001	0	3847	104	0
1	B	3999	0	3853	112	0
1	C	3993	0	3844	90	0
1	D	3993	0	3844	137	0
1	E	3993	0	3844	95	0
1	F	4001	0	3857	114	0
1	G	4001	0	3857	124	0
1	H	4001	0	3857	123	0
1	I	3993	0	3844	120	0
1	J	3991	0	3838	115	0
1	K	4001	0	3857	110	0
1	L	4001	0	3857	146	0
2	A	53	0	31	5	0
2	B	53	0	31	4	0
2	C	53	0	31	6	0
2	D	53	0	31	12	0
2	E	53	0	31	6	0
2	F	53	0	31	5	0
2	G	53	0	31	4	0
2	H	53	0	31	7	0
2	I	53	0	31	5	0
2	J	53	0	31	7	0
2	K	53	0	31	6	0
2	L	53	0	31	5	0
All	All	48604	0	46571	1381	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 15.

All (1381) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:GLY:O	1:C:253:GLU:HG2	1.25	1.28
1:K:58:THR:HG22	1:K:214:HIS:CE1	1.70	1.26
1:B:375:ASN:N	1:B:376:SER:HB2	1.56	1.21
1:F:80:ASP:OD1	1:F:101:ARG:NH2	1.75	1.20
1:L:377:ASP:HB3	1:L:378:SER:O	1.42	1.19
1:K:11:TYR:OH	1:K:198:ASP:OD2	1.62	1.15
1:G:381[A]:ARG:HG3	1:G:381[A]:ARG:HH11	1.08	1.14
1:B:375:ASN:H	1:B:376:SER:CB	1.62	1.13
1:I:374:LEU:HA	1:I:375:ASN:HB2	1.17	1.13
1:L:376:SER:OG	1:L:377:ASP:HB2	1.50	1.11
1:B:196:ALA:HB1	1:B:197:SER:HB3	1.12	1.10
1:C:31:ILE:HD13	1:C:255:ILE:HG21	1.26	1.09
1:H:377:ASP:N	1:H:378:SER:HA	1.51	1.09
1:L:196:ALA:HB1	1:L:197:SER:HB3	1.13	1.09
1:G:196:ALA:HB1	1:G:197:SER:CB	1.83	1.08
1:J:377:ASP:H	1:J:378:SER:CA	1.67	1.07
1:L:376:SER:CB	1:L:377:ASP:HB2	1.85	1.07
1:J:377:ASP:H	1:J:378:SER:HA	1.20	1.06
1:C:252:GLY:O	1:C:253:GLU:CG	2.06	1.03
1:L:379:ASP:HB3	1:L:382:VAL:HG23	1.37	1.03
1:F:206:PRO:HG3	1:L:6:ASP:OD2	1.57	1.03
1:J:196:ALA:HB1	1:J:197:SER:CB	1.87	1.02
1:L:377:ASP:H	1:L:378:SER:HA	1.22	1.01
1:D:9:PHE:HB3	1:D:12:LEU:HD12	1.42	1.01
1:H:60:PRO:HB3	1:H:108:MET:HE2	1.44	0.99
1:E:377:ASP:N	1:E:378:SER:HB2	1.77	0.98
1:B:196:ALA:HB1	1:B:197:SER:CB	1.92	0.98
1:J:196:ALA:HB1	1:J:197:SER:HB2	1.43	0.98
1:G:196:ALA:HB1	1:G:197:SER:HB3	0.99	0.97
1:J:60:PRO:HB3	1:J:108:MET:HE2	1.44	0.97
1:F:21:LEU:HD11	1:F:212:ALA:HB2	1.47	0.96
1:G:196:ALA:CB	1:G:197:SER:HB3	1.93	0.96
1:D:21:LEU:HD11	1:D:212:ALA:CB	1.95	0.96
1:E:66:LEU:HD13	1:E:108:MET:HG3	1.47	0.96
1:I:374:LEU:HA	1:I:375:ASN:CB	1.94	0.96
1:K:11:TYR:CZ	1:K:198:ASP:OD2	2.19	0.95
1:D:41:LEU:HD21	1:D:255:ILE:HG12	1.52	0.92
1:G:325:ASN:O	1:G:364:PRO:HD2	1.70	0.92
1:L:196:ALA:HB1	1:L:197:SER:CB	1.98	0.92
1:C:196:ALA:HB1	1:C:197:SER:HB3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PRO:HB3	1:B:108:MET:HE2	1.50	0.91
1:H:376:SER:C	1:H:378:SER:HB2	1.95	0.91
1:F:252:GLY:C	1:F:253:GLU:HG2	1.95	0.91
1:A:21:LEU:HD11	1:A:212:ALA:HB2	1.53	0.91
1:I:374:LEU:CA	1:I:375:ASN:HB2	1.98	0.91
1:H:377:ASP:N	1:H:378:SER:CA	2.33	0.90
1:G:376:SER:HB2	1:G:377:ASP:HB2	1.52	0.90
1:E:326:PHE:HA	1:E:364:PRO:HD3	1.52	0.90
1:K:106:THR:O	1:K:108:MET:N	2.05	0.90
1:G:376:SER:CB	1:G:377:ASP:HB2	2.02	0.89
1:D:100:GLY:H	1:D:106:THR:HG23	1.38	0.89
1:L:377:ASP:H	1:L:378:SER:CA	1.85	0.89
1:C:21:LEU:HD11	1:C:212:ALA:CB	2.02	0.88
1:H:58:THR:HG22	1:H:214:HIS:NE2	1.88	0.88
1:C:255:ILE:O	1:C:255:ILE:HG22	1.71	0.88
1:K:58:THR:HG22	1:K:214:HIS:HE1	1.32	0.88
1:C:60:PRO:HB3	1:C:108:MET:HE2	1.56	0.87
1:H:376:SER:O	1:H:378:SER:HB2	1.75	0.87
1:G:381[A]:ARG:HG3	1:G:381[A]:ARG:NH1	1.84	0.86
1:L:249[B]:ARG:HH11	1:L:249[B]:ARG:HB3	1.40	0.86
1:G:58:THR:HG22	1:G:214:HIS:CE1	2.11	0.86
1:C:31:ILE:HA	1:C:255:ILE:HG22	1.58	0.86
1:B:279:SER:C	1:B:281:LEU:H	1.84	0.85
1:C:252:GLY:C	1:C:253:GLU:CG	2.46	0.85
1:D:198:ASP:OD1	1:D:199:GLU:N	2.09	0.85
1:L:196:ALA:CB	1:L:197:SER:HB3	2.04	0.84
1:F:44:THR:HG23	1:F:508:ARG:NH1	1.93	0.84
1:C:31:ILE:HA	1:C:255:ILE:CG2	2.08	0.84
1:H:325:ASN:O	1:H:364:PRO:HD3	1.78	0.84
1:I:9:PHE:HB3	1:I:12:LEU:HD12	1.60	0.83
1:C:252:GLY:C	1:C:253:GLU:HG2	2.03	0.83
1:C:486:VAL:HG21	1:C:510:VAL:HG11	1.60	0.83
1:H:41:LEU:HD21	1:H:255:ILE:HG21	1.60	0.83
1:F:101:ARG:O	1:F:101:ARG:HG2	1.80	0.82
1:B:31:ILE:HB	1:B:53:VAL:HG13	1.60	0.82
1:H:376:SER:O	1:H:378:SER:CB	2.28	0.81
1:L:376:SER:OG	1:L:377:ASP:CB	2.27	0.81
1:B:58:THR:HG22	1:B:59:LEU:H	1.45	0.81
1:J:9:PHE:HB3	1:J:12:LEU:HD12	1.62	0.81
1:J:196:ALA:CB	1:J:197:SER:HB2	2.10	0.81
1:B:375:ASN:H	1:B:376:SER:HB2	0.70	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:LEU:HD11	1:L:212:ALA:HB1	1.63	0.80
1:C:255:ILE:O	1:C:255:ILE:CG2	2.29	0.80
1:J:196:ALA:HB1	1:J:197:SER:HB3	1.62	0.80
1:C:31:ILE:HD13	1:C:255:ILE:CG2	2.09	0.80
1:I:325:ASN:O	1:I:364:PRO:HD2	1.81	0.80
1:L:389:ASN:HB3	1:L:392:SER:HB2	1.64	0.80
1:G:377:ASP:O	1:G:378:SER:HB2	1.79	0.80
1:I:268:LEU:HD13	1:I:374:LEU:HD21	1.62	0.80
1:H:376:SER:OG	1:H:378:SER:CA	2.30	0.80
1:B:21:LEU:HD11	1:B:212:ALA:HB2	1.64	0.80
1:D:346:ASN:OD1	1:D:348:THR:HG23	1.80	0.80
1:H:376:SER:OG	1:H:378:SER:HA	1.80	0.80
1:K:221:ILE:HD11	1:K:235:ILE:HG13	1.64	0.79
1:F:80:ASP:CG	1:F:101:ARG:HH22	1.88	0.79
1:L:48[B]:LYS:HD2	1:L:48[B]:LYS:O	1.81	0.79
1:G:44:THR:OG1	1:G:508:ARG:HG3	1.83	0.79
1:L:458:TYR:HD2	1:L:460:HIS:CD2	2.00	0.79
1:D:486:VAL:HG21	1:D:510:VAL:HG11	1.64	0.79
1:L:58:THR:HG23	1:L:214:HIS:CE1	2.17	0.79
1:B:196:ALA:CB	1:B:197:SER:HB3	2.05	0.78
1:B:41:LEU:HD21	1:B:255:ILE:HG21	1.64	0.78
1:B:58:THR:HG23	1:B:214:HIS:CE1	2.18	0.78
1:H:376:SER:C	1:H:378:SER:CB	2.57	0.78
1:J:414:ASP:HA	1:J:417:LYS:HG3	1.65	0.78
1:D:21:LEU:HD11	1:D:212:ALA:HB2	1.63	0.77
1:J:376:SER:HA	1:J:377:ASP:HB2	1.66	0.77
1:L:401:VAL:HG22	1:L:447:PHE:HB3	1.65	0.77
1:D:107:SER:OG	1:D:197:SER:OG	2.02	0.77
1:H:376:SER:C	1:H:378:SER:HA	2.09	0.77
1:L:377:ASP:CB	1:L:378:SER:O	2.30	0.77
1:B:86:VAL:HG22	1:B:109:ILE:HD13	1.66	0.77
1:L:142:GLU:HA	1:L:146:VAL:HG23	1.66	0.76
1:J:58:THR:HG22	1:J:214:HIS:CE1	2.20	0.76
1:G:389:ASN:HB3	1:G:392:SER:OG	1.85	0.76
1:D:110:ASN:HB2	2:D:773:FAD:C5X	2.16	0.76
1:B:9:PHE:HB3	1:B:12:LEU:HD12	1.67	0.76
1:A:80:ASP:OD1	1:A:101:ARG:NH2	2.19	0.76
1:D:227:SER:O	1:D:228:GLY:C	2.29	0.76
1:C:370:GLY:HA3	1:C:387:LYS:O	1.87	0.75
1:I:374:LEU:CA	1:I:375:ASN:CB	2.62	0.75
1:I:197:SER:OG	1:I:504:LEU:HD21	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:372:ILE:CD1	1:I:384:PRO:HB2	2.14	0.75
1:E:377:ASP:CA	1:E:378:SER:HB2	2.17	0.75
1:J:21:LEU:HD11	1:J:212:ALA:CB	2.16	0.75
1:J:21:LEU:HD11	1:J:212:ALA:HB1	1.67	0.75
1:L:127:ILE:HD11	1:L:129:TRP:CD2	2.21	0.75
1:G:58:THR:HG22	1:G:214:HIS:NE2	2.02	0.75
1:A:421:VAL:HG21	1:A:431:ASP:HB2	1.69	0.75
1:J:153:ALA:HB3	1:J:313:GLU:OE2	1.87	0.74
1:L:21:LEU:HD11	1:L:212:ALA:CB	2.16	0.74
1:C:389:ASN:HB3	1:C:392:SER:OG	1.86	0.74
1:D:367:LEU:HD22	1:F:521:ALA:HA	1.70	0.74
1:D:157:LEU:HD11	1:D:419:TYR:CZ	2.23	0.74
1:G:41:LEU:HD21	1:G:255:ILE:HG21	1.69	0.74
1:K:375:ASN:O	1:K:376:SER:HB3	1.87	0.74
1:B:227:SER:O	1:B:228:GLY:C	2.30	0.74
1:L:370:GLY:HA3	1:L:387:LYS:O	1.88	0.73
1:D:157:LEU:HD11	1:D:419:TYR:OH	1.87	0.73
1:G:252:GLY:C	1:G:253:GLU:HG2	2.12	0.73
1:I:327:TYR:OH	1:I:364:PRO:HB3	1.88	0.73
1:B:389:ASN:HB3	1:B:392:SER:OG	1.88	0.73
1:A:21:LEU:HD11	1:A:212:ALA:CB	2.18	0.73
1:H:21:LEU:HD11	1:H:212:ALA:HB2	1.70	0.73
1:E:420:LYS:HE2	1:E:430:PHE:CE1	2.24	0.73
1:F:370:GLY:HA3	1:F:387:LYS:O	1.88	0.73
1:E:325:ASN:O	1:E:364:PRO:HD2	1.89	0.73
1:A:508:ARG:HG3	1:A:508:ARG:HH11	1.53	0.72
1:E:107:SER:HG	1:E:197:SER:HG	1.34	0.72
1:E:488:GLY:HA2	1:E:503:TYR:CE2	2.24	0.72
1:H:252:GLY:O	1:H:253:GLU:HG2	1.87	0.72
1:D:29:TYR:HA	1:D:253:GLU:O	1.88	0.72
1:H:376:SER:C	1:H:378:SER:CA	2.62	0.72
1:I:414:ASP:OD2	1:I:417:LYS:HE2	1.90	0.72
1:D:58:THR:HG23	1:D:214:HIS:CE1	2.24	0.72
1:E:41:LEU:HD21	1:E:255:ILE:HG21	1.71	0.72
1:B:144:THR:OG1	1:B:203:LYS:HE2	1.89	0.72
1:D:106:THR:OG1	2:D:773:FAD:O1A	2.08	0.72
1:L:378:SER:O	1:L:379:ASP:HB2	1.89	0.72
1:D:44:THR:OG1	1:D:508:ARG:HG3	1.90	0.71
1:E:29:TYR:HA	1:E:253:GLU:O	1.90	0.71
1:B:279:SER:O	1:B:281:LEU:N	2.24	0.71
1:E:21:LEU:HD11	1:E:212:ALA:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD11	1:B:419:TYR:HE1	1.53	0.71
1:I:197:SER:OG	1:I:504:LEU:CD2	2.39	0.71
1:F:252:GLY:O	1:F:253:GLU:HG2	1.91	0.71
1:H:41:LEU:CD2	1:H:255:ILE:HG21	2.20	0.71
1:A:486:VAL:O	1:A:487:ASP:HB3	1.89	0.71
1:F:101:ARG:O	1:F:101:ARG:CG	2.39	0.71
1:C:110:ASN:HB2	2:C:773:FAD:C5X	2.20	0.70
1:G:421:VAL:HG21	1:G:431:ASP:HB2	1.72	0.70
1:I:110:ASN:HB2	2:I:773:FAD:N5	2.06	0.70
1:J:377:ASP:N	1:J:378:SER:CA	2.49	0.70
1:L:110:ASN:HB2	2:L:773:FAD:C5X	2.21	0.70
1:E:110:ASN:HB2	2:E:773:FAD:C5X	2.21	0.70
1:E:37:SER:O	1:E:40:PRO:HD2	1.92	0.70
1:F:327:TYR:OH	1:F:364:PRO:HB3	1.92	0.70
1:D:229:VAL:O	1:D:480:ILE:HG23	1.90	0.70
1:E:60:PRO:HB3	1:E:108:MET:HE2	1.73	0.70
1:J:387:LYS:NZ	1:J:389:ASN:OD1	2.20	0.70
1:D:218:GLU:OE2	1:D:237:LYS:HD2	1.90	0.70
1:G:127:ILE:HD11	1:G:129:TRP:CD2	2.27	0.70
1:F:41:LEU:HD21	1:F:255:ILE:HG21	1.74	0.70
1:D:100:GLY:N	1:D:106:THR:HG23	2.05	0.70
1:A:325:ASN:O	1:A:364:PRO:CD	2.40	0.69
1:L:458:TYR:CD2	1:L:460:HIS:CD2	2.79	0.69
1:I:372:ILE:HD11	1:I:384:PRO:HB2	1.74	0.69
1:I:41:LEU:HD21	1:I:255:ILE:HG21	1.75	0.69
1:F:58:THR:HG23	1:F:214:HIS:CE1	2.28	0.69
1:H:226:SER:HA	1:H:227:SER:O	1.93	0.69
1:B:21:LEU:HD11	1:B:212:ALA:CB	2.22	0.69
1:K:289:HIS:HB3	1:K:292:VAL:HG23	1.74	0.69
1:D:41:LEU:HD21	1:D:255:ILE:CG1	2.23	0.68
1:K:367:LEU:HD12	1:K:395:THR:HB	1.75	0.68
1:L:458:TYR:HD2	1:L:460:HIS:NE2	1.91	0.68
1:A:41:LEU:HD21	1:A:255:ILE:HG21	1.76	0.68
1:J:196:ALA:CA	1:J:197:SER:HB2	2.24	0.68
1:J:301:ARG:HD2	1:J:360:VAL:HG11	1.76	0.68
1:J:377:ASP:N	1:J:378:SER:HA	2.02	0.68
1:D:157:LEU:HD11	1:D:419:TYR:CE1	2.28	0.68
1:K:73:ILE:O	1:K:77:GLN:HG3	1.92	0.68
1:A:60:PRO:HB3	1:A:108:MET:HE2	1.76	0.68
1:E:301:ARG:HD2	1:E:360:VAL:HG11	1.76	0.68
1:G:376:SER:CB	1:G:377:ASP:CB	2.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ASP:OD1	1:H:101:ARG:NH2	2.25	0.68
1:F:101:ARG:HH11	1:F:381[B]:ARG:NH2	1.92	0.68
1:F:218:GLU:OE2	1:F:237:LYS:HD2	1.95	0.67
1:L:133:LEU:HD23	1:L:509:TYR:CD1	2.30	0.67
1:B:327:TYR:OH	1:B:364:PRO:HB3	1.95	0.67
1:F:101:ARG:HH11	1:F:381[B]:ARG:HH22	1.41	0.67
1:B:377:ASP:CB	1:B:378:SER:CA	2.72	0.67
1:G:69:SER:HB3	1:G:188:PHE:CE2	2.30	0.67
1:G:325:ASN:O	1:G:364:PRO:CD	2.43	0.67
1:H:421:VAL:HG21	1:H:431:ASP:HB2	1.76	0.67
1:J:301:ARG:HD2	1:J:360:VAL:CG1	2.24	0.67
1:E:110:ASN:HB2	2:E:773:FAD:N5	2.09	0.67
1:B:377:ASP:HB2	1:B:378:SER:CA	2.25	0.66
1:E:346:ASN:OD1	1:E:348:THR:HG22	1.95	0.66
1:H:393:ASN:HA	1:H:394:SER:HB2	1.78	0.66
1:I:236:TYR:CZ	1:I:244:HIS:HB2	2.30	0.66
1:I:303:PHE:HB3	1:I:360:VAL:HG12	1.77	0.66
1:L:459:TRP:HB3	2:L:773:FAD:HM82	1.76	0.66
1:D:325:ASN:O	1:D:364:PRO:HD2	1.95	0.66
1:I:74:TYR:HA	1:I:77:GLN:OE1	1.95	0.66
1:I:221:ILE:HD11	1:I:235:ILE:HG13	1.77	0.66
1:K:106:THR:C	1:K:108:MET:H	2.04	0.66
1:B:86:VAL:HG22	1:B:109:ILE:CD1	2.26	0.66
1:H:376:SER:OG	1:H:379:ASP:N	2.29	0.66
1:D:86:VAL:HG22	1:D:109:ILE:HD13	1.78	0.66
1:H:110:ASN:HB2	2:H:773:FAD:N5	2.10	0.66
1:H:358:HIS:CD2	1:H:360:VAL:HG13	2.30	0.66
1:I:325:ASN:O	1:I:364:PRO:CD	2.44	0.66
1:F:325:ASN:O	1:F:364:PRO:CD	2.43	0.65
1:F:206:PRO:CG	1:L:6:ASP:OD2	2.40	0.65
1:L:303:PHE:HA	1:L:359:PHE:O	1.95	0.65
1:H:63:TYR:O	1:H:66:LEU:HG	1.97	0.65
1:B:370:GLY:HA3	1:B:387:LYS:O	1.96	0.65
1:F:6:ASP:OD1	1:L:206:PRO:HG3	1.95	0.65
1:K:7:HIS:NE2	1:K:198:ASP:OD1	2.25	0.65
1:J:377:ASP:H	1:J:378:SER:C	2.05	0.65
1:D:260:PRO:HG3	1:D:488:GLY:O	1.96	0.65
1:G:196:ALA:CB	1:G:197:SER:CB	2.64	0.65
1:A:325:ASN:O	1:A:364:PRO:HD3	1.96	0.65
1:K:54:LEU:HD23	1:K:212:ALA:HB3	1.78	0.65
1:G:377:ASP:O	1:G:378:SER:CB	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:THR:O	1:K:107:SER:C	2.38	0.65
1:A:269:LEU:HD22	1:A:378:SER:HA	1.78	0.65
1:D:293:GLY:CA	1:D:372:ILE:HG22	2.27	0.64
1:D:294:GLN:O	1:D:464:GLY:HA2	1.97	0.64
1:I:301:ARG:HB2	1:I:458:TYR:CD1	2.32	0.64
1:K:106:THR:C	1:K:108:MET:N	2.55	0.64
1:L:9:PHE:HB3	1:L:12:LEU:HD12	1.78	0.64
1:F:21:LEU:HD11	1:F:212:ALA:CB	2.25	0.64
1:H:363:VAL:HG13	1:H:364:PRO:HD2	1.79	0.64
1:J:63:TYR:O	1:J:66:LEU:HG	1.97	0.64
1:L:376:SER:HB2	1:L:377:ASP:HB2	1.77	0.64
1:B:258:ALA:O	1:B:262:GLY:HA3	1.98	0.64
1:D:238:ASP:OD2	1:D:242:THR:HB	1.98	0.64
1:D:140:TRP:CE3	1:D:508:ARG:HD2	2.33	0.64
1:D:370:GLY:HA3	1:D:387:LYS:O	1.97	0.64
1:L:378:SER:OG	1:L:379:ASP:N	2.29	0.64
1:L:476:ARG:HA	1:L:484:ARG:HG2	1.80	0.64
1:D:80:ASP:OD1	1:D:101:ARG:NH2	2.26	0.63
1:G:195:HIS:C	1:G:196:ALA:O	2.30	0.63
1:K:327:TYR:OH	1:K:364:PRO:HB3	1.98	0.63
1:C:499:PRO:HB2	1:C:503:TYR:CE1	2.34	0.63
1:D:294:GLN:HB3	1:D:295:PHE:CD2	2.33	0.63
1:B:110:ASN:HB2	2:B:773:FAD:N5	2.13	0.63
1:I:499:PRO:HB2	1:I:503:TYR:CE1	2.33	0.63
1:D:106:THR:OG1	2:D:773:FAD:PA	2.57	0.63
1:D:293:GLY:HA2	1:D:372:ILE:HG22	1.81	0.63
1:C:140:TRP:CE2	1:C:203:LYS:HD3	2.34	0.62
1:F:29:TYR:HA	1:F:253:GLU:O	1.98	0.62
1:E:107:SER:OG	1:E:197:SER:OG	2.11	0.62
1:H:9:PHE:HB3	1:H:12:LEU:HD12	1.81	0.62
1:H:327:TYR:CZ	1:H:364:PRO:HB3	2.33	0.62
1:D:269:LEU:HD22	1:D:378:SER:HA	1.80	0.62
1:F:325:ASN:O	1:F:364:PRO:HD3	1.98	0.62
1:I:58:THR:HG23	1:I:214:HIS:CE1	2.33	0.62
1:I:198:ASP:OD1	1:I:199:GLU:N	2.32	0.62
1:B:173:PHE:HD1	1:B:183:LEU:O	1.82	0.62
1:G:118:ASN:O	1:G:121:ILE:HG22	2.00	0.62
1:H:341:PHE:O	1:H:342:ALA:HB3	1.98	0.62
1:J:334:LEU:HB3	1:J:335:PRO:HD2	1.82	0.62
1:A:358:HIS:CD2	1:A:360:VAL:HG13	2.34	0.62
1:K:291:TYR:CD1	1:K:469:GLU:HG3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:157:LEU:HD11	1:L:419:TYR:CE1	2.34	0.62
1:D:21:LEU:HD11	1:D:212:ALA:HB1	1.77	0.62
1:G:341:PHE:O	1:G:342:ALA:HB3	2.00	0.62
1:G:459:TRP:HB3	2:G:773:FAD:C8M	2.30	0.62
1:B:153:ALA:HB3	1:B:313:GLU:OE2	2.00	0.61
1:L:458:TYR:CD2	1:L:460:HIS:NE2	2.69	0.61
1:D:236:TYR:CZ	1:D:244:HIS:HB2	2.35	0.61
1:A:303:PHE:HB3	1:A:360:VAL:HG12	1.83	0.61
1:G:110:ASN:HB2	2:G:773:FAD:N5	2.16	0.61
1:L:157:LEU:HD11	1:L:419:TYR:HE1	1.65	0.61
1:G:236:TYR:CZ	1:G:244:HIS:HB2	2.35	0.61
1:H:218:GLU:OE2	1:H:237:LYS:HD2	1.99	0.61
1:B:327:TYR:CZ	1:B:364:PRO:HB3	2.36	0.61
1:D:106:THR:OG1	2:D:773:FAD:O2A	2.19	0.61
1:J:313:GLU:O	1:J:313:GLU:HG2	2.00	0.61
1:B:196:ALA:CB	1:B:197:SER:CB	2.73	0.60
1:J:65:ASN:O	1:J:71:GLY:HA3	2.02	0.60
1:J:110:ASN:HB2	2:J:773:FAD:N5	2.16	0.60
1:L:142:GLU:HA	1:L:146:VAL:CG2	2.31	0.60
1:L:377:ASP:N	1:L:378:SER:HA	2.05	0.60
1:D:108:MET:HE3	1:D:194:ARG:HD2	1.82	0.60
1:K:325:ASN:O	1:K:364:PRO:HD2	2.00	0.60
1:D:499:PRO:HB2	1:D:503:TYR:CE1	2.36	0.60
1:B:303:PHE:HA	1:B:359:PHE:O	2.01	0.60
1:J:144:THR:HG22	1:J:145:ILE:HG23	1.83	0.60
1:E:370:GLY:HA3	1:E:387:LYS:O	2.01	0.60
1:E:422:GLU:HG2	1:E:429:GLY:HA2	1.82	0.60
1:G:21:LEU:HD11	1:G:212:ALA:HB2	1.84	0.60
1:F:157:LEU:HD13	1:F:419:TYR:OH	2.02	0.60
1:D:358:HIS:CD2	1:D:360:VAL:HG13	2.37	0.60
1:J:459:TRP:HB3	2:J:773:FAD:C8	2.32	0.59
1:E:9:PHE:HB3	1:E:12:LEU:CD1	2.32	0.59
1:H:253:GLU:OE1	1:H:484:ARG:NE	2.31	0.59
1:L:144:THR:HG22	1:L:145:ILE:HG23	1.84	0.59
1:H:236:TYR:CZ	1:H:244:HIS:HB2	2.38	0.59
1:K:162:PHE:HB3	1:K:181:THR:OG1	2.02	0.59
1:C:252:GLY:C	1:C:253:GLU:HG3	2.26	0.59
1:D:260:PRO:HA	1:D:489:SER:HB3	1.84	0.59
1:L:320:LEU:HD23	1:L:329:CYS:HB3	1.84	0.59
1:A:327:TYR:OH	1:A:364:PRO:HB3	2.02	0.59
1:C:21:LEU:HD11	1:C:212:ALA:HB1	1.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ILE:HD11	1:C:437:LEU:HG	1.83	0.59
1:H:252:GLY:C	1:H:253:GLU:CG	2.75	0.59
1:J:27:TYR:O	1:J:248:VAL:HA	2.02	0.59
1:J:252:GLY:C	1:J:253:GLU:HG2	2.25	0.59
1:J:80:ASP:OD1	1:J:101:ARG:NH2	2.23	0.59
1:C:63:TYR:O	1:C:66:LEU:HG	2.02	0.59
1:G:110:ASN:HB2	2:G:773:FAD:C5X	2.33	0.59
1:H:56:ARG:HB2	1:H:381[B]:ARG:NH2	2.17	0.59
1:D:252:GLY:C	1:D:253:GLU:HG2	2.28	0.59
1:E:54:LEU:HD23	1:E:212:ALA:HB3	1.84	0.59
1:I:273:GLY:HA2	1:I:289:HIS:O	2.03	0.59
1:B:421:VAL:HG21	1:B:431:ASP:HB2	1.84	0.58
1:D:459:TRP:HB3	2:D:773:FAD:C8	2.33	0.58
1:G:127:ILE:HD11	1:G:129:TRP:CE2	2.38	0.58
1:A:48[A]:LYS:HE3	1:A:49:TYR:CE1	2.37	0.58
1:I:41:LEU:CD2	1:I:255:ILE:HG21	2.32	0.58
1:B:326:PHE:HA	1:B:364:PRO:HD3	1.84	0.58
1:I:301:ARG:HB2	1:I:458:TYR:HD1	1.67	0.58
1:K:177:HIS:HE1	1:K:327:TYR:CE2	2.22	0.58
1:H:376:SER:OG	1:H:377:ASP:N	2.37	0.58
1:A:140:TRP:CE3	1:A:508:ARG:HD2	2.38	0.58
1:H:252:GLY:O	1:H:253:GLU:CG	2.51	0.58
1:H:414:ASP:HA	1:H:417:LYS:HG3	1.85	0.58
1:I:21:LEU:HD11	1:I:212:ALA:CB	2.34	0.58
1:J:304:ILE:HG21	1:J:411:LEU:HD11	1.85	0.58
1:G:296:LEU:HD21	1:G:372:ILE:HG13	1.86	0.58
1:J:236:TYR:CZ	1:J:244:HIS:HB2	2.39	0.58
1:K:252:GLY:O	1:K:253:GLU:HG2	2.04	0.58
1:A:341:PHE:O	1:A:342:ALA:HB3	2.03	0.58
1:C:31:ILE:CD1	1:C:255:ILE:HG21	2.17	0.58
1:C:254:VAL:O	1:C:483:LEU:HA	2.04	0.58
1:G:499:PRO:HB2	1:G:503:TYR:CE1	2.38	0.58
1:I:136:GLN:O	1:I:139:ASP:HB2	2.03	0.58
1:J:463:GLY:H	1:J:489:SER:HA	1.69	0.58
1:J:241:GLY:O	1:J:243:PRO:HD3	2.03	0.58
1:L:155:GLN:HB3	1:L:319:VAL:HG23	1.85	0.58
1:D:110:ASN:HB2	2:D:773:FAD:N5	2.18	0.57
1:I:157:LEU:HD11	1:I:419:TYR:CE1	2.38	0.57
1:B:6:ASP:OD1	1:D:206:PRO:HG3	2.04	0.57
1:H:49:TYR:O	1:H:208:ASN:HB3	2.04	0.57
1:K:160:THR:HA	1:K:163:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ARG:HD2	1:C:360:VAL:HG11	1.85	0.57
1:G:9:PHE:HB3	1:G:12:LEU:HD12	1.84	0.57
1:I:263:SER:HB2	1:I:264:PRO:HD3	1.86	0.57
1:J:157:LEU:CD2	1:J:419:TYR:HE1	2.18	0.57
1:J:376:SER:CA	1:J:377:ASP:HB2	2.33	0.57
1:L:56:ARG:HG2	2:L:773:FAD:C4A	2.34	0.57
1:L:229:VAL:HG11	1:L:286:VAL:HG12	1.84	0.57
1:G:299:ASN:OD1	1:G:366:PRO:HD3	2.03	0.57
1:H:421:VAL:CG2	1:H:431:ASP:HB2	2.34	0.57
1:H:500:GLN:O	1:H:501:GLY:C	2.48	0.57
1:J:110:ASN:HB2	2:J:773:FAD:C5X	2.35	0.57
1:K:11:TYR:CE2	1:K:198:ASP:OD2	2.55	0.57
1:H:269:LEU:HD21	1:H:378:SER:HB3	1.85	0.57
1:H:325:ASN:O	1:H:364:PRO:CD	2.49	0.57
1:K:21:LEU:HD11	1:K:212:ALA:HB2	1.85	0.57
1:C:261:ILE:HG23	1:C:384:PRO:HG2	1.87	0.57
1:H:110:ASN:HB2	2:H:773:FAD:C5X	2.35	0.57
1:H:116:ARG:NH2	1:H:142:GLU:OE2	2.36	0.57
1:B:66:LEU:HD13	1:B:108:MET:HE3	1.85	0.57
1:F:263:SER:HB2	1:F:264:PRO:HD3	1.87	0.57
1:H:96:ASP:OD2	1:H:346:ASN:HA	2.04	0.57
1:L:271:GLY:HA3	1:L:286:VAL:HG23	1.86	0.57
1:B:29:TYR:HA	1:B:253:GLU:O	2.05	0.57
1:E:44:THR:OG1	1:E:508:ARG:HG3	2.04	0.57
1:K:352:PRO:HG3	1:K:356:PHE:CE2	2.40	0.57
1:L:327:TYR:OH	1:L:364:PRO:HB3	2.05	0.56
1:B:27:TYR:O	1:B:248:VAL:HA	2.05	0.56
1:D:41:LEU:CD2	1:D:255:ILE:HG12	2.30	0.56
1:G:186:SER:OG	1:G:188:PHE:HB2	2.05	0.56
1:H:333:SER:HB3	1:H:356:PHE:CE2	2.40	0.56
1:I:372:ILE:HD11	1:I:384:PRO:CB	2.35	0.56
1:L:294:GLN:O	1:L:295:PHE:HB2	2.04	0.56
1:C:196:ALA:HB3	1:C:198:ASP:OD1	2.04	0.56
1:D:12:LEU:HD21	1:D:59:LEU:HD13	1.87	0.56
1:E:66:LEU:HD13	1:E:108:MET:CG	2.30	0.56
1:G:2:ALA:HB3	1:G:147:TYR:CE1	2.40	0.56
1:G:226:SER:HA	1:G:227:SER:C	2.31	0.56
1:K:358:HIS:CD2	1:K:360:VAL:HG13	2.40	0.56
1:L:252:GLY:O	1:L:482:ALA:HB1	2.05	0.56
1:E:9:PHE:HB3	1:E:12:LEU:HD12	1.87	0.56
1:F:101:ARG:NH1	1:F:381[B]:ARG:NH2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ASP:OD1	1:I:206:PRO:HG3	2.05	0.56
1:H:331:PHE:CE2	1:H:333:SER:HB2	2.40	0.56
1:A:132:ASP:O	1:A:136:GLN:HB2	2.06	0.56
1:B:325:ASN:O	1:B:364:PRO:HD2	2.06	0.56
1:F:406:LYS:O	1:F:409:GLU:HB2	2.05	0.56
1:J:136:GLN:O	1:J:139:ASP:HB2	2.06	0.56
1:J:370:GLY:HA3	1:J:387:LYS:O	2.05	0.56
1:J:463:GLY:O	1:J:489:SER:HB2	2.04	0.56
1:K:252:GLY:C	1:K:253:GLU:CG	2.77	0.56
1:D:63:TYR:O	1:D:66:LEU:HG	2.06	0.56
1:F:260:PRO:HG3	1:F:462:HIS:HA	1.86	0.56
1:K:307:LEU:HD11	1:K:433:LEU:HB2	1.86	0.56
1:L:155:GLN:HB3	1:L:319:VAL:CG2	2.36	0.56
1:G:376:SER:CA	1:G:377:ASP:HB2	2.35	0.56
1:J:260:PRO:HA	1:J:489:SER:HB3	1.88	0.56
1:L:336:PHE:HB2	1:L:351:LEU:HD22	1.88	0.56
1:D:326:PHE:HA	1:D:364:PRO:HD3	1.86	0.56
1:K:236:TYR:CZ	1:K:244:HIS:HB2	2.41	0.56
1:E:377:ASP:HB2	1:E:378:SER:OG	2.06	0.56
1:F:221:ILE:HB	1:F:232:ILE:HG13	1.87	0.56
1:K:27:TYR:O	1:K:248:VAL:HA	2.06	0.56
1:H:58:THR:HG22	1:H:214:HIS:CE1	2.42	0.55
1:H:377:ASP:H	1:H:378:SER:HA	1.63	0.55
1:C:327:TYR:OH	1:C:364:PRO:HB3	2.06	0.55
1:E:331:PHE:CE2	1:E:333:SER:HB2	2.41	0.55
1:I:69:SER:HB3	1:I:188:PHE:CD2	2.41	0.55
1:C:106:THR:HB	2:C:773:FAD:O4'	2.06	0.55
1:F:289:HIS:HB3	1:F:292:VAL:HG23	1.88	0.55
1:A:463:GLY:H	1:A:489:SER:HA	1.71	0.55
1:C:358:HIS:CD2	1:C:360:VAL:HG13	2.42	0.55
1:H:376:SER:OG	1:H:378:SER:CB	2.55	0.55
1:K:314:PRO:HA	1:K:332:SER:O	2.06	0.55
1:A:302:ASN:OD1	1:A:391:TYR:OH	2.22	0.55
1:F:261:ILE:HG23	1:F:384:PRO:HG2	1.88	0.55
1:J:116:ARG:HG2	1:J:138:TYR:CD2	2.41	0.55
1:B:411:LEU:HB3	1:B:430:PHE:CE1	2.42	0.55
1:H:370:GLY:HA3	1:H:387:LYS:O	2.06	0.55
1:F:304:ILE:HD11	1:F:437:LEU:HG	1.89	0.55
1:G:29:TYR:HA	1:G:253:GLU:O	2.07	0.55
1:K:236:TYR:CE1	1:K:244:HIS:HB2	2.42	0.55
1:L:515:LEU:O	1:L:519:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:HD21	1:D:255:ILE:CD1	2.37	0.55
1:L:376:SER:CB	1:L:377:ASP:CB	2.74	0.55
1:L:376:SER:CA	1:L:377:ASP:HB2	2.37	0.55
1:L:331:PHE:HB3	1:L:358:HIS:HB3	1.89	0.55
1:G:29:TYR:HB2	1:G:51:VAL:HG22	1.89	0.54
1:G:72:PHE:CD2	1:G:73:ILE:HD13	2.42	0.54
1:G:196:ALA:CA	1:G:197:SER:CB	2.85	0.54
1:K:66:LEU:O	1:K:194:ARG:HD2	2.07	0.54
1:A:160:THR:O	1:A:164:GLU:HG3	2.06	0.54
1:G:27:TYR:CE1	1:G:52:LEU:HD22	2.42	0.54
1:G:44:THR:O	1:G:47:GLU:HB2	2.08	0.54
1:D:458:TYR:O	1:D:459:TRP:HB2	2.08	0.54
1:F:401:VAL:HG22	1:F:447:PHE:HB3	1.90	0.54
1:H:327:TYR:OH	1:H:364:PRO:HB3	2.06	0.54
1:I:269:LEU:HD22	1:I:378:SER:HA	1.88	0.54
1:I:301:ARG:HD2	1:I:360:VAL:HG11	1.88	0.54
1:A:174:SER:O	1:A:182:ARG:HD2	2.07	0.54
1:A:326:PHE:HE2	1:A:402:SER:HB3	1.71	0.54
1:E:499:PRO:HB2	1:E:503:TYR:CE1	2.42	0.54
1:L:196:ALA:CB	1:L:197:SER:CB	2.76	0.54
1:L:377:ASP:N	1:L:378:SER:C	2.66	0.54
1:A:459:TRP:HB3	2:A:773:FAD:C8M	2.37	0.54
1:B:228:GLY:O	1:B:229:VAL:C	2.49	0.54
1:C:236:TYR:CZ	1:C:244:HIS:CB	2.89	0.54
1:C:236:TYR:CZ	1:C:244:HIS:HB2	2.42	0.54
1:D:463:GLY:O	1:D:489:SER:HB2	2.07	0.54
1:G:269:LEU:HD22	1:G:378:SER:HA	1.88	0.54
1:H:226:SER:HA	1:H:227:SER:C	2.31	0.54
1:A:127:ILE:HG13	1:A:128:GLU:N	2.22	0.54
1:B:41:LEU:CD2	1:B:255:ILE:HG21	2.36	0.54
1:H:393:ASN:HA	1:H:394:SER:CB	2.35	0.54
1:I:110:ASN:HB2	2:I:773:FAD:C5X	2.37	0.54
1:K:305:ASN:HB2	1:K:433:LEU:O	2.08	0.54
1:D:236:TYR:CE1	1:D:244:HIS:HB2	2.42	0.54
1:F:376:SER:O	1:F:377:ASP:C	2.50	0.54
1:G:80:ASP:OD1	1:G:101:ARG:NH2	2.37	0.54
1:D:255:ILE:CD1	1:D:486:VAL:HG23	2.37	0.54
1:F:393:ASN:HA	1:F:394:SER:OG	2.08	0.54
1:H:11:TYR:OH	1:H:198:ASP:OD2	2.06	0.53
1:L:66:LEU:HD13	1:L:108:MET:HG3	1.89	0.53
1:A:101:ARG:HH11	1:A:381:ARG:HH22	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:VAL:CG2	1:D:510:VAL:HG11	2.35	0.53
1:G:236:TYR:CE2	1:G:244:HIS:HB2	2.44	0.53
1:A:294:GLN:O	1:A:464:GLY:HA2	2.09	0.53
1:I:39:CYS:N	1:I:40:PRO:HD2	2.23	0.53
1:I:132:ASP:O	1:I:136:GLN:HB2	2.07	0.53
1:H:60:PRO:HD3	1:H:103:LEU:HB3	1.91	0.53
1:A:260:PRO:O	1:A:264:PRO:HG2	2.08	0.53
1:D:60:PRO:HD3	1:D:103:LEU:HB3	1.90	0.53
1:D:313:GLU:CD	1:D:313:GLU:H	2.14	0.53
1:I:9:PHE:HB3	1:I:12:LEU:CD1	2.33	0.53
1:F:195:HIS:HA	1:F:199:GLU:OE1	2.07	0.53
1:J:291:TYR:CD1	1:J:469:GLU:HG3	2.44	0.53
1:L:88:ARG:HB3	1:L:341:PHE:CE2	2.42	0.53
1:D:290:PRO:HA	1:F:128:GLU:HG2	1.91	0.53
1:D:297:HIS:HB3	1:D:366:PRO:HD2	1.91	0.53
1:G:329:CYS:O	1:G:360:VAL:HG22	2.09	0.53
1:G:376:SER:OG	1:G:377:ASP:CB	2.57	0.53
1:H:27:TYR:CE1	1:H:52:LEU:HD22	2.44	0.53
1:K:359:PHE:HZ	1:K:416:LEU:HD11	1.74	0.53
1:A:343:PHE:HA	1:A:459:TRP:HZ2	1.73	0.53
1:D:227:SER:C	1:D:228:GLY:O	2.51	0.53
1:K:21:LEU:HD11	1:K:212:ALA:CB	2.39	0.53
1:K:162:PHE:HZ	1:K:328:GLN:HB3	1.73	0.53
1:B:297:HIS:HB3	1:B:366:PRO:HD2	1.91	0.53
1:B:58:THR:HG22	1:B:59:LEU:N	2.21	0.53
1:B:134:VAL:HG13	1:B:505:MET:HE2	1.91	0.53
1:F:110:ASN:HB2	2:F:773:FAD:N5	2.24	0.53
1:F:265:GLN:NE2	1:F:384:PRO:HD3	2.23	0.53
1:G:376:SER:OG	1:G:377:ASP:HB3	2.08	0.53
1:L:377:ASP:H	1:L:378:SER:C	2.15	0.53
1:A:299:ASN:ND2	1:A:366:PRO:HD3	2.25	0.52
1:C:297:HIS:HB3	1:C:366:PRO:HD2	1.90	0.52
1:G:142:GLU:HA	1:G:146:VAL:HG23	1.91	0.52
1:J:35:GLY:HA3	2:J:773:FAD:O5B	2.09	0.52
1:J:488:GLY:HA2	1:J:503:TYR:CE2	2.44	0.52
1:B:107:SER:OG	1:B:197:SER:CB	2.57	0.52
1:D:48[B]:LYS:HD2	1:D:48[B]:LYS:O	2.09	0.52
1:L:27:TYR:CE1	1:L:52:LEU:HD22	2.43	0.52
1:A:162:PHE:HB3	1:A:181:THR:OG1	2.08	0.52
1:D:325:ASN:O	1:D:364:PRO:CD	2.58	0.52
1:E:252:GLY:C	1:E:253:GLU:HG2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:157:LEU:CD1	1:L:419:TYR:OH	2.58	0.52
1:D:121:ILE:C	1:D:123:SER:H	2.18	0.52
1:J:301:ARG:HG3	1:J:360:VAL:HG12	1.91	0.52
1:J:377:ASP:N	1:J:378:SER:C	2.67	0.52
1:K:56:ARG:HG2	2:K:773:FAD:C4A	2.39	0.52
1:K:269:LEU:HD22	1:K:378:SER:HA	1.91	0.52
1:K:306:ILE:HG13	1:K:357:ALA:HB3	1.92	0.52
1:K:358:HIS:CD2	1:K:360:VAL:CG1	2.93	0.52
1:K:404:MET:HB3	1:K:437:LEU:HD21	1.91	0.52
1:A:110:ASN:HB2	2:A:773:FAD:C5X	2.40	0.52
1:A:486:VAL:O	1:A:487:ASP:CB	2.58	0.52
1:B:3:THR:O	1:B:4:THR:C	2.53	0.52
1:B:459:TRP:HB3	2:B:773:FAD:C8M	2.40	0.52
1:C:420:LYS:HE2	1:C:428:ASP:O	2.10	0.52
1:E:102:VAL:HG11	1:E:108:MET:HB3	1.92	0.52
1:B:162:PHE:CE2	1:B:410:LEU:HD21	2.44	0.52
1:I:513:LYS:O	1:I:517:GLU:HG2	2.10	0.52
1:C:196:ALA:CB	1:C:197:SER:HB3	2.31	0.52
1:E:6:ASP:OD1	1:H:206:PRO:HG3	2.09	0.52
1:I:475:PHE:CZ	1:I:506:LEU:HD11	2.44	0.52
1:L:375:ASN:O	1:L:376:SER:CB	2.57	0.52
1:A:54:LEU:HD23	1:A:212:ALA:HB3	1.92	0.52
1:D:140:TRP:CD2	1:D:508:ARG:HD2	2.44	0.52
1:G:381[A]:ARG:NH1	1:G:381[A]:ARG:CG	2.61	0.52
1:K:375:ASN:O	1:K:376:SER:CB	2.58	0.52
1:A:99:ARG:HB3	1:A:461:TYR:OH	2.09	0.52
1:A:508:ARG:HG3	1:A:508:ARG:NH1	2.22	0.52
1:D:144:THR:HG22	1:D:145:ILE:HG23	1.91	0.52
1:E:486:VAL:O	1:E:487:ASP:HB3	2.09	0.52
1:I:341:PHE:O	1:I:342:ALA:HB3	2.10	0.52
1:J:41:LEU:HD21	1:J:255:ILE:HG21	1.91	0.52
1:J:65:ASN:ND2	1:J:74:TYR:CE2	2.78	0.52
1:L:11:TYR:HB2	1:L:14:PHE:CE1	2.44	0.52
1:B:110:ASN:HB2	2:B:773:FAD:C5X	2.39	0.52
1:D:157:LEU:CD1	1:D:419:TYR:OH	2.57	0.52
1:K:297:HIS:HB3	1:K:366:PRO:HD2	1.91	0.52
1:L:346:ASN:ND2	1:L:348:THR:HG23	2.25	0.51
1:J:17:ASP:HA	1:J:213:VAL:HG23	1.92	0.51
1:L:41:LEU:HD21	1:L:255:ILE:HG21	1.91	0.51
1:F:421:VAL:N	1:F:429:GLY:O	2.42	0.51
1:G:17:ASP:OD2	1:G:19:THR:OG1	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:PHE:HZ	1:G:416:LEU:HD11	1.76	0.51
1:H:303:PHE:HA	1:H:359:PHE:O	2.11	0.51
1:E:301:ARG:HG3	1:E:360:VAL:HG12	1.92	0.51
1:F:69:SER:C	1:F:71:GLY:H	2.19	0.51
1:I:158:THR:HG21	1:I:330:SER:HB3	1.92	0.51
1:L:236:TYR:CZ	1:L:244:HIS:HB2	2.46	0.51
1:A:499:PRO:HB2	1:A:503:TYR:CE1	2.46	0.51
1:B:173:PHE:CD1	1:B:183:LEU:O	2.62	0.51
1:D:352:PRO:HG3	1:D:433:LEU:CD2	2.41	0.51
1:E:89:PHE:CZ	1:E:97:ASP:HB3	2.46	0.51
1:G:45:LEU:C	1:G:47:GLU:H	2.18	0.51
1:K:359:PHE:CZ	1:K:416:LEU:HD11	2.46	0.51
1:L:306:ILE:O	1:L:308:PRO:HD3	2.10	0.51
1:C:9:PHE:HB3	1:C:12:LEU:CD1	2.40	0.51
1:E:167:VAL:HG12	1:E:180:GLY:HA2	1.92	0.51
1:J:260:PRO:HG3	1:J:488:GLY:O	2.11	0.51
1:J:325:ASN:O	1:J:364:PRO:HD2	2.10	0.51
1:K:325:ASN:HB3	1:K:399:HIS:CD2	2.45	0.51
1:L:27:TYR:CE2	1:L:52:LEU:HB2	2.45	0.51
1:E:127:ILE:HG22	1:E:473:GLY:HA2	1.93	0.51
1:E:327:TYR:CZ	1:E:364:PRO:HG3	2.46	0.51
1:H:56:ARG:HB2	1:H:381[B]:ARG:HH22	1.75	0.51
1:J:196:ALA:CB	1:J:197:SER:CB	2.73	0.51
1:K:18:ALA:HB2	1:K:215:ALA:HB2	1.91	0.51
1:K:71:GLY:O	1:K:74:TYR:N	2.44	0.51
1:K:438:PRO:HG2	1:K:447:PHE:CD1	2.46	0.51
1:F:363:VAL:HG13	1:F:364:PRO:HD2	1.92	0.51
1:F:450:PHE:C	1:F:450:PHE:CD2	2.88	0.51
1:K:71:GLY:O	1:K:72:PHE:C	2.53	0.51
1:A:218:GLU:OE2	1:A:237:LYS:HD2	2.10	0.51
1:F:179:ALA:HA	1:F:322:ILE:HG22	1.93	0.51
1:F:416:LEU:HB3	1:F:430:PHE:HZ	1.76	0.51
1:A:326:PHE:CE2	1:A:402:SER:HB3	2.46	0.51
1:B:303:PHE:CB	1:B:358:HIS:CE1	2.94	0.51
1:F:47:GLU:O	1:F:48[B]:LYS:HD2	2.11	0.51
1:H:12:LEU:HD21	1:H:59:LEU:HD22	1.93	0.51
1:H:346:ASN:HB2	1:H:347:PRO:HD2	1.93	0.51
1:I:268:LEU:HD13	1:I:374:LEU:CD2	2.39	0.51
1:B:228:GLY:O	1:B:229:VAL:O	2.29	0.50
1:B:499:PRO:HB2	1:B:503:TYR:CE1	2.46	0.50
1:C:362:LYS:HB2	1:C:458:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:THR:O	1:D:164:GLU:HG3	2.11	0.50
1:D:498:HIS:HB3	2:D:773:FAD:O2	2.10	0.50
1:L:168:LEU:HB3	1:L:169:PRO:HA	1.92	0.50
1:A:260:PRO:HA	1:A:489:SER:HB3	1.92	0.50
1:F:73:ILE:O	1:F:77:GLN:HG3	2.10	0.50
1:K:260:PRO:CG	1:K:462:HIS:HA	2.40	0.50
1:B:60:PRO:HB3	1:B:108:MET:CE	2.32	0.50
1:E:291:TYR:CD1	1:E:469:GLU:HG3	2.46	0.50
1:G:189:ASP:O	1:G:192:GLY:N	2.40	0.50
1:H:21:LEU:HD11	1:H:212:ALA:CB	2.40	0.50
1:H:500:GLN:HG2	2:H:773:FAD:O2	2.12	0.50
1:B:303:PHE:HB2	1:B:358:HIS:CE1	2.47	0.50
1:B:328:GLN:OE1	1:B:407:ILE:HG13	2.10	0.50
1:C:337:SER:OG	1:C:338:ILE:HD12	2.11	0.50
1:E:43:ALA:O	1:E:46:SER:OG	2.29	0.50
1:K:305:ASN:CB	1:K:433:LEU:HB3	2.41	0.50
1:L:463:GLY:O	1:L:489:SER:HA	2.11	0.50
1:B:463:GLY:O	1:B:489:SER:HA	2.11	0.50
1:E:301:ARG:HD2	1:E:360:VAL:CG1	2.42	0.50
1:G:145:ILE:HG22	1:G:195:HIS:HB3	1.93	0.50
1:I:337:SER:C	1:I:338:ILE:HG13	2.37	0.50
1:K:205:ASP:C	1:K:205:ASP:OD1	2.53	0.50
1:A:69:SER:HB3	1:A:188:PHE:CD2	2.47	0.50
1:A:122:PHE:O	1:A:129:TRP:CD1	2.64	0.50
1:E:467:VAL:HG23	1:E:490:THR:O	2.11	0.50
1:F:111:ALA:HB3	2:F:773:FAD:O4	2.12	0.50
1:H:368:SER:HB3	1:H:392:SER:HB2	1.94	0.50
1:J:328:GLN:NE2	1:J:403:GLY:O	2.44	0.50
1:L:66:LEU:HD12	1:L:66:LEU:C	2.36	0.50
1:L:469:GLU:N	1:L:469:GLU:OE1	2.45	0.50
1:A:444:ASP:O	1:A:448:GLU:HG3	2.12	0.50
1:C:58:THR:HG23	1:C:214:HIS:CE1	2.47	0.50
1:F:197:SER:HB3	1:F:504:LEU:CD2	2.41	0.50
1:L:196:ALA:CA	1:L:197:SER:CB	2.90	0.50
1:L:366:PRO:HB2	1:L:396:ASP:OD2	2.12	0.50
1:A:370:GLY:HA3	1:A:387:LYS:O	2.12	0.50
1:C:256:VAL:HG23	1:C:484:ARG:O	2.12	0.50
1:E:194:ARG:HG2	1:E:195:HIS:N	2.27	0.50
1:F:197:SER:HB3	1:F:504:LEU:HD21	1.94	0.50
1:H:397:LEU:HD22	1:H:452:ARG:NH2	2.27	0.50
1:I:189:ASP:C	1:I:189:ASP:OD2	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:GLU:OE2	1:I:237:LYS:HD2	2.12	0.50
1:L:252:GLY:O	1:L:253:GLU:HG2	2.10	0.50
1:L:404:MET:HE2	1:L:450:PHE:HE2	1.77	0.50
1:I:417:LYS:N	1:I:418:PRO:CD	2.75	0.50
1:J:297:HIS:HB3	1:J:366:PRO:HD2	1.93	0.50
1:A:80:ASP:HB2	1:A:88:ARG:HG3	1.94	0.49
1:D:459:TRP:HB3	2:D:773:FAD:C8M	2.42	0.49
1:D:471:LEU:HD11	1:D:490:THR:HG22	1.93	0.49
1:F:458:TYR:O	1:F:459:TRP:HB2	2.11	0.49
1:G:353:ASN:O	1:J:354:SER:HA	2.13	0.49
1:I:404:MET:HG3	1:I:450:PHE:CE2	2.46	0.49
1:J:127:ILE:HG12	1:J:129:TRP:CE2	2.46	0.49
1:K:110:ASN:HB2	2:K:773:FAD:N5	2.27	0.49
1:L:98:VAL:O	1:L:461:TYR:OH	2.23	0.49
1:D:358:HIS:CD2	1:D:360:VAL:CG1	2.95	0.49
1:G:107:SER:OG	1:G:197:SER:HB2	2.12	0.49
1:G:326:PHE:HA	1:G:364:PRO:HD3	1.93	0.49
1:G:404:MET:HG3	1:G:450:PHE:HE2	1.77	0.49
1:I:110:ASN:HB2	2:I:773:FAD:C4X	2.42	0.49
1:J:363:VAL:HG12	1:J:364:PRO:O	2.12	0.49
1:L:114:TYR:C	1:L:114:TYR:CD2	2.90	0.49
1:L:375:ASN:OD1	1:L:375:ASN:N	2.43	0.49
1:B:195:HIS:C	1:B:196:ALA:O	2.52	0.49
1:K:404:MET:HE2	1:K:450:PHE:HE2	1.77	0.49
1:D:198:ASP:OD1	1:D:198:ASP:N	2.41	0.49
1:G:63:TYR:O	1:G:65:ASN:N	2.46	0.49
1:A:142:GLU:C	1:A:144:THR:H	2.21	0.49
1:E:1:LEU:HD13	1:E:148:LYS:HB2	1.94	0.49
1:G:142:GLU:HA	1:G:146:VAL:CG2	2.43	0.49
1:B:157:LEU:CD1	1:B:419:TYR:HE1	2.24	0.49
1:C:238:ASP:OD2	1:C:242:THR:HB	2.13	0.49
1:D:296:LEU:HD12	1:D:388:PHE:HE2	1.78	0.49
1:I:236:TYR:CE1	1:I:244:HIS:HB2	2.47	0.49
1:I:372:ILE:HD11	1:I:384:PRO:CG	2.43	0.49
1:K:302:ASN:ND2	1:K:400:CYS:SG	2.86	0.49
1:B:227:SER:O	1:B:228:GLY:O	2.30	0.49
1:E:326:PHE:HA	1:E:364:PRO:CD	2.35	0.49
1:F:301:ARG:HB2	1:F:458:TYR:CD1	2.47	0.49
1:A:325:ASN:O	1:A:364:PRO:HD2	2.12	0.49
1:D:488:GLY:HA2	1:D:503:TYR:CE2	2.47	0.49
1:F:136:GLN:O	1:F:139:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:326:PHE:HA	1:J:364:PRO:HD3	1.95	0.49
1:K:499:PRO:HD2	2:K:773:FAD:N1	2.28	0.49
1:A:102:VAL:HG11	1:A:108:MET:HB3	1.95	0.49
1:C:15:ALA:HA	1:C:211:VAL:O	2.13	0.49
1:F:499:PRO:HB2	1:F:503:TYR:CE1	2.48	0.49
1:H:197:SER:HA	1:H:200:LEU:HG	1.95	0.49
1:I:22:GLU:CD	1:I:22:GLU:H	2.20	0.49
1:I:73:ILE:HD12	1:I:336:PHE:CE2	2.48	0.49
1:I:108:MET:HE3	1:I:194:ARG:HD2	1.95	0.49
1:K:363:VAL:HG12	1:K:364:PRO:O	2.13	0.49
1:A:320:LEU:HD23	1:A:329:CYS:HB3	1.95	0.48
1:D:197:SER:HB3	1:D:504:LEU:HD21	1.95	0.48
1:F:60:PRO:HB3	1:F:108:MET:HE2	1.95	0.48
1:I:411:LEU:HB3	1:I:430:PHE:CE1	2.48	0.48
1:C:103:LEU:HD21	1:C:211:VAL:HG11	1.95	0.48
1:A:379:ASP:HB3	1:A:382:VAL:HG23	1.95	0.48
1:D:27:TYR:O	1:D:248:VAL:HA	2.12	0.48
1:D:222:PHE:HA	1:D:230:THR:O	2.14	0.48
1:D:227:SER:O	1:D:228:GLY:O	2.30	0.48
1:E:238:ASP:OD1	1:E:238:ASP:C	2.57	0.48
1:F:236:TYR:CZ	1:F:244:HIS:HB3	2.48	0.48
1:H:121:ILE:HD13	1:H:121:ILE:O	2.13	0.48
1:H:378:SER:OG	1:H:379:ASP:C	2.57	0.48
1:C:110:ASN:HB2	2:C:773:FAD:N5	2.28	0.48
1:H:222:PHE:CD1	1:H:286:VAL:HG11	2.49	0.48
1:I:313:GLU:CD	1:I:313:GLU:H	2.21	0.48
1:I:458:TYR:O	1:I:459:TRP:HB2	2.13	0.48
1:J:499:PRO:HB2	1:J:503:TYR:CE1	2.48	0.48
1:K:136:GLN:O	1:K:139:ASP:HB3	2.14	0.48
1:K:326:PHE:HA	1:K:364:PRO:HD3	1.95	0.48
1:K:487:ASP:OD2	1:K:489:SER:N	2.46	0.48
1:A:48[A]:LYS:HE3	1:A:49:TYR:HE1	1.78	0.48
1:E:37:SER:C	1:E:40:PRO:HD2	2.37	0.48
1:F:54:LEU:HD23	1:F:212:ALA:HB3	1.95	0.48
1:G:236:TYR:CZ	1:G:244:HIS:CB	2.97	0.48
1:G:249:ARG:O	1:G:250:GLY:C	2.57	0.48
1:I:237:LYS:HE3	1:I:241:GLY:O	2.14	0.48
1:K:336:PHE:H	1:K:352:PRO:HG2	1.78	0.48
1:L:11:TYR:OH	1:L:198:ASP:OD2	2.24	0.48
1:E:127:ILE:HD11	1:E:129:TRP:CZ2	2.48	0.48
1:H:341:PHE:O	1:H:342:ALA:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:304:ILE:HD11	1:L:437:LEU:HG	1.94	0.48
1:A:260:PRO:HG3	1:A:462:HIS:HA	1.94	0.48
1:F:284:PRO:HG3	1:K:282:ASN:HB2	1.96	0.48
1:G:10:SER:HB2	1:G:202:ASN:OD1	2.13	0.48
1:H:252:GLY:C	1:H:253:GLU:HG3	2.38	0.48
1:H:376:SER:CB	1:H:378:SER:HB2	2.44	0.48
1:F:69:SER:C	1:F:71:GLY:N	2.72	0.48
1:B:225:ASN:HA	1:B:227:SER:HA	1.96	0.48
1:B:279:SER:C	1:B:281:LEU:N	2.51	0.48
1:E:104:GLY:O	1:E:107:SER:OG	2.32	0.48
1:F:360:VAL:HG21	1:F:458:TYR:OH	2.14	0.48
1:C:472:ASP:OD1	1:C:476:ARG:N	2.47	0.48
1:D:133:LEU:HD23	1:D:509:TYR:CE1	2.49	0.48
1:F:40:PRO:HB3	1:F:200:LEU:HD13	1.95	0.48
1:G:67:LEU:HD23	1:G:108:MET:CE	2.44	0.48
1:H:156:SER:O	1:H:160:THR:HG23	2.14	0.48
1:H:488:GLY:HA2	1:H:503:TYR:CZ	2.49	0.48
1:L:459:TRP:HB3	2:L:773:FAD:C8M	2.44	0.48
1:A:48[B]:LYS:HD2	1:A:48[B]:LYS:HA	1.67	0.47
1:B:336:PHE:HB2	1:B:351:LEU:HD22	1.96	0.47
1:C:254:VAL:HA	1:C:255:ILE:HB	1.94	0.47
1:C:420:LYS:HE3	1:C:430:PHE:CE1	2.48	0.47
1:E:116:ARG:HG2	1:E:138:TYR:CD2	2.49	0.47
1:G:299:ASN:ND2	1:G:362:LYS:HE2	2.29	0.47
1:H:50:LYS:HD3	1:H:208:ASN:HA	1.95	0.47
1:H:161:ALA:HB2	1:H:415:ALA:HB3	1.96	0.47
1:K:156:SER:O	1:K:159:LYS:HB3	2.14	0.47
1:B:401:VAL:HG22	1:B:447:PHE:HB3	1.96	0.47
1:J:137:THR:HG23	1:J:508:ARG:HD3	1.96	0.47
1:J:401:VAL:HG12	1:J:405:LYS:HE3	1.96	0.47
1:C:153:ALA:HB3	1:C:313:GLU:CD	2.40	0.47
1:C:487:ASP:OD2	1:C:487:ASP:C	2.57	0.47
1:D:198:ASP:OD1	1:D:198:ASP:C	2.40	0.47
1:E:136:GLN:O	1:E:139:ASP:HB2	2.15	0.47
1:I:372:ILE:HG12	1:I:386:VAL:HG12	1.96	0.47
1:J:157:LEU:HD13	1:J:419:TYR:OH	2.14	0.47
1:K:260:PRO:HA	1:K:489:SER:HB3	1.95	0.47
1:A:342:ALA:HB1	1:A:459:TRP:HE1	1.79	0.47
1:J:196:ALA:HA	1:J:197:SER:HB2	1.96	0.47
1:A:22:GLU:OE1	1:A:210:ARG:NH2	2.48	0.47
1:A:66:LEU:HD13	1:A:108:MET:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LEU:HD11	1:C:433:LEU:HB2	1.97	0.47
1:D:153:ALA:HB3	1:D:313:GLU:HG3	1.97	0.47
1:D:331:PHE:HB3	1:D:358:HIS:HB3	1.96	0.47
1:F:21:LEU:CD1	1:F:212:ALA:CB	2.90	0.47
1:F:41:LEU:CD2	1:F:255:ILE:HG21	2.40	0.47
1:G:226:SER:HA	1:G:227:SER:O	2.15	0.47
1:H:85:PRO:HA	1:H:101:ARG:O	2.15	0.47
1:H:269:LEU:CD2	1:H:378:SER:HB3	2.43	0.47
1:I:63:TYR:O	1:I:66:LEU:HG	2.13	0.47
1:J:411:LEU:HB3	1:J:430:PHE:CE1	2.50	0.47
1:K:405:LYS:N	1:K:447:PHE:HE2	2.12	0.47
1:A:274:PRO:HG3	1:A:290:PRO:O	2.14	0.47
1:A:304:ILE:HD11	1:A:437:LEU:HG	1.96	0.47
1:C:110:ASN:O	1:C:194:ARG:NH1	2.31	0.47
1:D:275:GLU:HB2	1:D:288:SER:OG	2.14	0.47
1:E:422:GLU:HG3	1:E:424:LEU:HG	1.96	0.47
1:F:365:GLY:HA2	1:F:493:TYR:HB3	1.96	0.47
1:F:459:TRP:HB3	2:F:773:FAD:C8	2.44	0.47
1:J:147:TYR:OH	1:J:195:HIS:CE1	2.68	0.47
1:J:471:LEU:HD13	1:J:475:PHE:HA	1.96	0.47
1:L:302:ASN:ND2	1:L:391:TYR:OH	2.37	0.47
1:L:404:MET:HE2	1:L:450:PHE:CE2	2.50	0.47
1:A:145:ILE:O	1:A:187:THR:HG22	2.15	0.47
1:A:162:PHE:CD2	1:A:410:LEU:HD11	2.48	0.47
1:E:408:GLY:HA2	1:E:411:LEU:HD12	1.96	0.47
1:E:500:GLN:HG2	2:E:773:FAD:O2	2.15	0.47
1:F:12:LEU:CD2	1:F:59:LEU:HD13	2.44	0.47
1:F:187:THR:HB	1:F:195:HIS:O	2.15	0.47
1:F:249:ARG:O	1:F:250:GLY:C	2.58	0.47
1:G:144:THR:OG1	1:G:203:LYS:HE2	2.14	0.47
1:H:113:VAL:HB	1:H:498:HIS:CD2	2.49	0.47
1:H:499:PRO:HB2	1:H:503:TYR:CE1	2.49	0.47
1:I:281:LEU:HD21	1:I:375:ASN:H	1.79	0.47
1:J:157:LEU:CD2	1:J:419:TYR:CE1	2.97	0.47
1:K:41:LEU:HD21	1:K:255:ILE:HG21	1.97	0.47
1:L:127:ILE:HD11	1:L:129:TRP:CE2	2.49	0.47
1:L:260:PRO:O	1:L:264:PRO:CD	2.63	0.47
1:C:32:VAL:HG13	1:C:217:VAL:HG21	1.97	0.47
1:D:226:SER:HA	1:D:227:SER:HA	1.53	0.47
1:F:32:VAL:HG13	1:F:217:VAL:HG21	1.97	0.47
1:F:200:LEU:O	1:F:203:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:PHE:CD1	1:G:286:VAL:HG11	2.50	0.47
1:G:296:LEU:CD2	1:G:372:ILE:HG13	2.45	0.47
1:K:440:ASN:HB3	1:K:443:ASP:HB2	1.97	0.47
1:L:122:PHE:O	1:L:129:TRP:HD1	1.98	0.47
1:L:379:ASP:HB3	1:L:382:VAL:CG2	2.25	0.47
1:B:27:TYR:N	1:B:27:TYR:CD1	2.83	0.47
1:D:144:THR:OG1	1:D:203:LYS:HE2	2.14	0.47
1:G:154:TRP:CZ3	1:G:157:LEU:HD22	2.50	0.47
1:H:73:ILE:HD12	1:H:336:PHE:CE2	2.49	0.47
1:I:31:ILE:HD13	1:I:255:ILE:HG13	1.96	0.47
1:J:157:LEU:HD21	1:J:419:TYR:HE1	1.79	0.47
1:J:327:TYR:OH	1:J:364:PRO:HB3	2.15	0.47
1:K:291:TYR:O	1:K:294:GLN:HB2	2.15	0.47
1:B:54:LEU:HD23	1:B:212:ALA:HB3	1.96	0.47
1:C:335:PRO:HG3	1:H:353:ASN:O	2.14	0.47
1:G:277:TYR:CZ	1:G:281:LEU:HD11	2.49	0.47
1:H:471:LEU:CD1	1:H:490:THR:HG22	2.44	0.47
1:L:56:ARG:NE	1:L:101:ARG:HG3	2.30	0.47
1:L:250:GLY:O	1:L:251:GLU:HB2	2.14	0.47
1:L:269:LEU:HD12	1:L:380:VAL:HG23	1.97	0.47
1:D:261:ILE:O	1:D:264:PRO:HD2	2.15	0.46
1:J:223:SER:C	1:J:225:ASN:H	2.23	0.46
1:L:196:ALA:HA	1:L:197:SER:HB2	1.98	0.46
1:B:261:ILE:HA	1:B:372:ILE:HD11	1.97	0.46
1:C:153:ALA:HB3	1:C:313:GLU:OE2	2.14	0.46
1:C:254:VAL:CA	1:C:255:ILE:HB	2.45	0.46
1:E:27:TYR:O	1:E:248:VAL:HA	2.15	0.46
1:F:21:LEU:CD1	1:F:212:ALA:HB2	2.31	0.46
1:G:189:ASP:C	1:G:189:ASP:OD2	2.57	0.46
1:I:297:HIS:HB3	1:I:366:PRO:HD2	1.97	0.46
1:J:158:THR:HG22	1:J:162:PHE:CE1	2.51	0.46
1:J:301:ARG:HB2	1:J:458:TYR:CD1	2.50	0.46
1:K:58:THR:HG22	1:K:214:HIS:NE2	2.23	0.46
1:A:339:PRO:HB3	1:A:351:LEU:HD21	1.97	0.46
1:E:299:ASN:CG	1:E:366:PRO:HD3	2.40	0.46
1:J:304:ILE:HD11	1:J:437:LEU:HG	1.96	0.46
1:B:98:VAL:HG13	1:B:342:ALA:HB2	1.97	0.46
1:B:116:ARG:NH2	1:B:142:GLU:OE1	2.49	0.46
1:B:255:ILE:HA	1:B:484:ARG:O	2.16	0.46
1:B:460:HIS:O	1:B:461:TYR:C	2.57	0.46
1:C:9:PHE:HB3	1:C:12:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASP:OD1	1:C:170:ASP:C	2.59	0.46
1:D:303:PHE:HB3	1:D:360:VAL:HG12	1.98	0.46
1:D:372:ILE:HG23	1:D:372:ILE:O	2.15	0.46
1:I:69:SER:C	1:I:71:GLY:H	2.23	0.46
1:I:222:PHE:CD1	1:I:286:VAL:HG11	2.50	0.46
1:I:369:TYR:CD1	1:I:369:TYR:C	2.93	0.46
1:K:320:LEU:HD23	1:K:329:CYS:HB3	1.96	0.46
1:G:360:VAL:HG21	1:G:458:TYR:OH	2.16	0.46
1:I:372:ILE:CD1	1:I:384:PRO:CB	2.90	0.46
1:J:249:ARG:O	1:J:250:GLY:C	2.59	0.46
1:L:230:THR:HG22	1:L:231:ALA:N	2.30	0.46
1:F:236:TYR:CZ	1:F:244:HIS:CB	2.99	0.46
1:G:282:ASN:HB2	1:K:284:PRO:HG3	1.98	0.46
1:I:127:ILE:HD11	1:I:129:TRP:CZ2	2.50	0.46
1:I:249:ARG:O	1:I:250:GLY:C	2.58	0.46
1:K:252:GLY:C	1:K:253:GLU:HG3	2.41	0.46
1:K:499:PRO:HD2	2:K:773:FAD:C2	2.45	0.46
1:L:220:ILE:HG13	1:L:270:SER:OG	2.16	0.46
1:A:358:HIS:CD2	1:A:360:VAL:CG1	2.99	0.46
1:F:107:SER:OG	1:F:196:ALA:HB1	2.15	0.46
1:F:248:VAL:HB	1:F:252:GLY:HA3	1.98	0.46
1:G:147:TYR:OH	1:G:195:HIS:CE1	2.68	0.46
1:K:404:MET:HE2	1:K:450:PHE:CE2	2.51	0.46
1:A:118:ASN:O	1:A:121:ILE:HB	2.15	0.46
1:J:48[B]:LYS:HE2	1:J:48[B]:LYS:O	2.16	0.46
1:J:174:SER:O	1:J:184:THR:HA	2.15	0.46
1:B:236:TYR:CZ	1:B:244:HIS:HB2	2.51	0.46
1:C:80:ASP:OD1	1:C:101:ARG:NH2	2.37	0.46
1:C:437:LEU:HD22	1:C:447:PHE:CE2	2.51	0.46
1:E:229:VAL:HG11	1:E:286:VAL:HG13	1.98	0.46
1:F:346:ASN:HB2	1:F:348:THR:HG22	1.97	0.46
1:K:353:ASN:O	1:L:335:PRO:HG3	2.15	0.46
1:L:152:GLN:O	1:L:153:ALA:C	2.57	0.46
1:L:299:ASN:ND2	1:L:366:PRO:HD3	2.31	0.46
1:E:48[A]:LYS:O	1:E:48[A]:LYS:HG3	2.16	0.46
1:E:117:ALA:HA	1:E:496:ALA:HB2	1.98	0.46
1:E:189:ASP:OD2	1:E:189:ASP:C	2.59	0.46
1:J:263:SER:HB2	1:J:264:PRO:HD3	1.97	0.46
1:K:341:PHE:O	1:K:342:ALA:HB3	2.16	0.46
1:L:377:ASP:N	1:L:378:SER:CA	2.55	0.46
1:A:458:TYR:O	1:A:459:TRP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:GLN:O	1:B:504:LEU:HG	2.17	0.45
1:E:325:ASN:O	1:E:364:PRO:CD	2.60	0.45
1:G:417:LYS:N	1:G:418:PRO:CD	2.79	0.45
1:G:459:TRP:HB3	2:G:773:FAD:HM81	1.98	0.45
1:L:56:ARG:HA	1:L:215:ALA:O	2.16	0.45
1:L:84:THR:HB	1:L:85:PRO:HD2	1.97	0.45
1:D:121:ILE:O	1:D:123:SER:N	2.49	0.45
1:D:303:PHE:HA	1:D:359:PHE:O	2.16	0.45
2:I:773:FAD:H9	2:I:773:FAD:H1'1	1.72	0.45
1:J:424:LEU:HB3	1:J:425:PRO:HD2	1.99	0.45
1:C:467:VAL:HA	1:C:471:LEU:HB2	1.98	0.45
1:E:377:ASP:CA	1:E:378:SER:CB	2.92	0.45
1:F:279:SER:C	1:F:281:LEU:H	2.24	0.45
1:H:260:PRO:HG3	1:H:462:HIS:HA	1.99	0.45
1:I:16:TYR:O	1:I:212:ALA:HA	2.17	0.45
1:I:404:MET:HG3	1:I:450:PHE:HE2	1.82	0.45
1:L:379:ASP:C	1:L:381:ARG:N	2.72	0.45
1:C:498:HIS:HB3	2:C:773:FAD:O2	2.17	0.45
1:D:499:PRO:HD2	2:D:773:FAD:N1	2.32	0.45
1:F:9:PHE:HZ	1:F:67:LEU:HD21	1.82	0.45
1:H:66:LEU:HD12	1:H:67:LEU:HG	1.99	0.45
1:J:261:ILE:HG23	1:J:384:PRO:HG2	1.98	0.45
1:K:127:ILE:HG12	1:K:129:TRP:CE2	2.51	0.45
1:L:138:TYR:HB3	1:L:142:GLU:OE2	2.16	0.45
1:F:353:ASN:O	1:I:335:PRO:HG3	2.16	0.45
1:H:477:VAL:CG1	1:H:480:ILE:HD12	2.46	0.45
1:I:486:VAL:HG21	1:I:510:VAL:HG11	1.99	0.45
1:A:472:ASP:OD1	1:A:472:ASP:C	2.60	0.45
1:D:255:ILE:HD11	1:D:486:VAL:HB	1.98	0.45
1:E:346:ASN:OD1	1:E:348:THR:CG2	2.64	0.45
1:F:435:ILE:HA	1:F:436:PRO:HD3	1.74	0.45
1:G:137:THR:HG23	1:G:508:ARG:HD3	1.99	0.45
1:H:488:GLY:HA2	1:H:503:TYR:CE2	2.51	0.45
1:I:21:LEU:HD11	1:I:212:ALA:HB2	1.99	0.45
1:K:7:HIS:CE1	1:K:199:GLU:OE1	2.68	0.45
1:D:291:TYR:O	1:D:294:GLN:HB2	2.16	0.45
1:E:287:LEU:HG	1:E:288:SER:N	2.32	0.45
1:H:307:LEU:HD11	1:H:433:LEU:HB2	1.98	0.45
1:I:127:ILE:HD11	1:I:129:TRP:CE2	2.52	0.45
1:I:127:ILE:HG22	1:I:473:GLY:HA2	1.99	0.45
1:J:459:TRP:HB3	2:J:773:FAD:C8M	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:VAL:O	1:B:487:ASP:HB3	2.16	0.45
1:D:307:LEU:HD11	1:D:433:LEU:HB2	1.99	0.45
1:E:229:VAL:HG11	1:E:286:VAL:CG1	2.47	0.45
1:E:231:ALA:HB3	1:E:482:ALA:O	2.16	0.45
1:G:341:PHE:O	1:G:342:ALA:CB	2.63	0.45
1:H:378:SER:OG	1:H:379:ASP:O	2.29	0.45
1:I:10:SER:HB2	1:I:202:ASN:OD1	2.17	0.45
1:L:54:LEU:HD23	1:L:212:ALA:HB3	1.98	0.45
1:L:225:ASN:HB3	1:L:226:SER:HB3	1.98	0.45
1:A:198:ASP:OD1	1:A:198:ASP:N	2.49	0.45
1:A:474:ASP:O	1:A:475:PHE:HB2	2.17	0.45
1:B:177:HIS:HA	1:B:182:ARG:NH1	2.32	0.45
1:D:513:LYS:O	1:D:517:GLU:HG2	2.17	0.45
1:H:299:ASN:CG	1:H:366:PRO:HD3	2.42	0.45
1:J:194:ARG:HG2	1:J:195:HIS:N	2.30	0.45
1:K:305:ASN:HB2	1:K:433:LEU:HB3	1.98	0.45
1:D:293:GLY:HA2	1:D:372:ILE:CG2	2.44	0.45
1:E:150:ASP:O	1:E:151:LYS:C	2.60	0.45
1:F:29:TYR:CE2	1:F:253:GLU:HG3	2.52	0.45
1:G:376:SER:CA	1:G:377:ASP:CB	2.95	0.45
1:H:127:ILE:HD11	1:H:129:TRP:CD2	2.52	0.45
1:I:225:ASN:HA	1:I:226:SER:HA	1.47	0.45
1:I:277:TYR:CE2	1:I:374:LEU:O	2.70	0.45
1:I:323:THR:HG22	1:I:324:SER:H	1.82	0.45
1:B:325:ASN:O	1:B:364:PRO:CD	2.65	0.44
1:B:389:ASN:HB3	1:B:392:SER:HG	1.81	0.44
1:I:198:ASP:OD1	1:I:198:ASP:N	2.48	0.44
1:K:177:HIS:CE1	1:K:327:TYR:CE2	3.05	0.44
1:K:256:VAL:HG12	1:K:263:SER:OG	2.17	0.44
1:L:162:PHE:HB3	1:L:181:THR:OG1	2.17	0.44
1:B:60:PRO:HD3	1:B:103:LEU:HB3	1.99	0.44
1:C:116:ARG:NH2	1:C:142:GLU:OE1	2.51	0.44
1:C:225:ASN:HA	1:C:226:SER:HA	1.72	0.44
1:D:281:LEU:HD12	1:D:377:ASP:HA	2.00	0.44
1:G:107:SER:OG	1:G:197:SER:CB	2.65	0.44
1:G:116:ARG:NH2	1:G:142:GLU:OE2	2.51	0.44
1:K:250:GLY:O	1:K:251:GLU:HB2	2.17	0.44
1:A:183:LEU:C	1:A:183:LEU:HD23	2.43	0.44
1:A:325:ASN:C	1:A:364:PRO:HD3	2.42	0.44
1:A:508:ARG:O	1:A:508:ARG:HG2	2.15	0.44
1:C:59:LEU:HD23	1:C:213:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:ASN:C	1:E:364:PRO:HG2	2.42	0.44
1:E:377:ASP:CB	1:E:378:SER:HB2	2.48	0.44
1:E:467:VAL:HA	1:E:471:LEU:HB2	1.99	0.44
1:G:45:LEU:C	1:G:47:GLU:N	2.76	0.44
1:I:106:THR:HG22	1:I:106:THR:O	2.17	0.44
1:I:157:LEU:C	1:I:157:LEU:HD23	2.43	0.44
1:I:274:PRO:HD3	1:I:289:HIS:O	2.18	0.44
1:J:306:ILE:HG12	1:J:357:ALA:HB3	2.00	0.44
1:K:142:GLU:C	1:K:144:THR:H	2.24	0.44
1:L:9:PHE:HB3	1:L:12:LEU:CD1	2.48	0.44
1:A:364:PRO:O	1:A:366:PRO:HA	2.17	0.44
1:B:118:ASN:HB3	1:B:121:ILE:HG12	1.99	0.44
1:C:27:TYR:CE1	1:C:52:LEU:HD22	2.52	0.44
1:C:474:ASP:O	1:C:475:PHE:HB2	2.17	0.44
1:D:229:VAL:HG11	1:D:286:VAL:HG12	1.99	0.44
1:D:379:ASP:C	1:D:381:ARG:N	2.74	0.44
1:E:377:ASP:HB2	1:E:378:SER:CB	2.47	0.44
1:I:238:ASP:C	1:I:238:ASP:OD1	2.60	0.44
1:K:305:ASN:ND2	1:K:349:TYR:OH	2.50	0.44
1:K:471:LEU:HA	1:K:476:ARG:O	2.17	0.44
1:K:505:MET:HB3	1:K:505:MET:HE3	1.70	0.44
1:L:110:ASN:HB2	2:L:773:FAD:N5	2.32	0.44
1:A:226:SER:HA	1:A:227:SER:HA	1.77	0.44
1:B:328:GLN:HA	1:B:360:VAL:O	2.17	0.44
1:D:422:GLU:HG3	1:D:424:LEU:HG	1.98	0.44
1:E:103:LEU:HD12	1:E:104:GLY:H	1.82	0.44
1:E:218:GLU:OE2	1:E:237:LYS:HD2	2.17	0.44
1:E:341:PHE:O	1:E:342:ALA:HB3	2.17	0.44
1:F:301:ARG:HB2	1:F:458:TYR:HD1	1.83	0.44
1:G:261:ILE:HG23	1:G:384:PRO:HG2	1.99	0.44
1:H:376:SER:OG	1:H:378:SER:HB2	2.17	0.44
1:H:467:VAL:HA	1:H:471:LEU:HB2	2.00	0.44
1:I:39:CYS:CB	1:I:197:SER:O	2.65	0.44
1:K:205:ASP:HA	1:K:206:PRO:HD2	1.82	0.44
1:L:49:TYR:O	1:L:208:ASN:HB3	2.17	0.44
1:A:268:LEU:HB3	1:A:374:LEU:HD11	1.99	0.44
1:B:327:TYR:HD1	1:B:362:LYS:HD3	1.81	0.44
1:D:16:TYR:O	1:D:212:ALA:HA	2.18	0.44
2:E:773:FAD:H9	2:E:773:FAD:H1'1	1.62	0.44
1:F:376:SER:O	1:F:378:SER:N	2.51	0.44
1:F:474:ASP:OD2	1:F:476:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:PRO:HA	1:H:489:SER:HB3	1.98	0.44
1:H:358:HIS:NE2	1:H:360:VAL:HG13	2.33	0.44
1:K:58:THR:CG2	1:K:214:HIS:CE1	2.67	0.44
1:L:269:LEU:CD1	1:L:380:VAL:HG23	2.48	0.44
1:B:196:ALA:CA	1:B:197:SER:CB	2.95	0.44
1:C:66:LEU:HD13	1:C:108:MET:HE3	2.00	0.44
1:G:148:LYS:HG3	1:G:173:PHE:CE1	2.52	0.44
1:G:306:ILE:HD13	1:G:359:PHE:HE2	1.83	0.44
1:A:142:GLU:C	1:A:144:THR:N	2.76	0.44
1:D:137:THR:HG23	1:D:508:ARG:HB3	2.00	0.44
1:D:474:ASP:O	1:D:475:PHE:HB2	2.17	0.44
1:E:459:TRP:HB3	2:E:773:FAD:C8M	2.48	0.44
1:G:60:PRO:HB3	1:G:108:MET:HE2	2.00	0.44
1:G:307:LEU:HD23	1:G:356:PHE:HB3	1.99	0.44
1:G:510:VAL:O	1:G:514:ILE:HG13	2.18	0.44
1:I:179:ALA:HA	1:I:322:ILE:O	2.17	0.44
1:I:364:PRO:O	1:I:366:PRO:HA	2.18	0.44
1:A:110:ASN:O	1:A:194:ARG:NH2	2.44	0.44
1:B:322:ILE:HD12	1:B:327:TYR:CD2	2.52	0.44
1:D:99:ARG:HB3	1:D:461:TYR:OH	2.17	0.44
1:F:377:ASP:O	1:F:378:SER:CB	2.66	0.44
1:G:352:PRO:HG3	1:G:356:PHE:CE2	2.53	0.44
1:H:229:VAL:HG11	1:H:286:VAL:CG1	2.48	0.44
1:L:249[B]:ARG:HH11	1:L:249[B]:ARG:CB	2.19	0.44
1:L:255:ILE:HG23	1:L:255:ILE:HD13	1.58	0.44
1:C:27:TYR:O	1:C:248:VAL:HA	2.18	0.43
1:C:301:ARG:HD2	1:C:360:VAL:CG1	2.48	0.43
1:F:162:PHE:CE2	1:F:410:LEU:HD11	2.52	0.43
1:F:376:SER:C	1:F:378:SER:N	2.76	0.43
1:G:73:ILE:HD13	1:G:73:ILE:N	2.33	0.43
1:H:110:ASN:HB2	2:H:773:FAD:C4X	2.47	0.43
1:I:248:VAL:HG11	1:I:253:GLU:H	1.82	0.43
1:I:300:PRO:HD2	1:I:363:VAL:HB	1.99	0.43
1:J:29:TYR:HE2	1:J:253:GLU:HG3	1.83	0.43
1:K:73:ILE:HG22	1:K:77:GLN:NE2	2.33	0.43
1:K:330:SER:HA	1:K:358:HIS:O	2.17	0.43
1:K:475:PHE:CZ	1:K:506:LEU:HD11	2.53	0.43
1:L:99:ARG:HB3	1:L:461:TYR:OH	2.18	0.43
1:A:471:LEU:HA	1:A:476:ARG:O	2.18	0.43
1:C:459:TRP:HB3	2:C:773:FAD:C8M	2.48	0.43
1:D:106:THR:O	1:D:110:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:HIS:HA	1:D:290:PRO:HD2	1.90	0.43
1:K:120:LYS:HA	1:K:120:LYS:HD2	1.77	0.43
1:A:341:PHE:O	1:A:342:ALA:CB	2.66	0.43
1:A:346:ASN:HB2	1:A:347:PRO:HD2	2.00	0.43
1:F:24:GLU:O	1:F:24:GLU:HG3	2.18	0.43
1:K:60:PRO:HB3	1:K:108:MET:HE2	2.00	0.43
1:L:32:VAL:HG13	1:L:217:VAL:HG21	2.00	0.43
1:A:111:ALA:HB3	2:A:773:FAD:O4	2.18	0.43
1:D:137:THR:HG23	1:D:508:ARG:HD3	1.99	0.43
1:F:252:GLY:O	1:F:253:GLU:CG	2.62	0.43
1:H:304:ILE:HG13	1:H:437:LEU:HG	2.00	0.43
1:I:301:ARG:HD3	1:I:458:TYR:CD1	2.53	0.43
1:I:363:VAL:HG12	1:I:364:PRO:O	2.18	0.43
1:I:511:GLY:HA2	1:I:514:ILE:HD12	2.00	0.43
1:J:60:PRO:HD3	1:J:103:LEU:HB3	2.00	0.43
1:K:110:ASN:HB2	2:K:773:FAD:C4X	2.48	0.43
1:K:110:ASN:HB2	2:K:773:FAD:C5X	2.49	0.43
1:L:225:ASN:HA	1:L:226:SER:HA	1.67	0.43
1:L:301:ARG:HB2	1:L:458:TYR:CD1	2.54	0.43
1:D:162:PHE:HD2	1:D:410:LEU:HD11	1.83	0.43
1:G:404:MET:HG3	1:G:450:PHE:CE2	2.53	0.43
1:I:24:GLU:HA	1:I:245:GLN:O	2.18	0.43
1:I:275:GLU:HG3	1:I:285:VAL:HG21	2.00	0.43
1:J:29:TYR:CE2	1:J:253:GLU:HG3	2.53	0.43
1:J:323:THR:HG22	1:J:324:SER:N	2.33	0.43
1:L:226:SER:HA	1:L:227:SER:HA	1.59	0.43
1:L:376:SER:HA	1:L:377:ASP:HA	1.53	0.43
1:A:4:THR:HG23	1:A:189:ASP:CG	2.44	0.43
1:C:31:ILE:HG23	1:C:255:ILE:HG23	2.00	0.43
1:D:58:THR:HG22	1:D:59:LEU:H	1.84	0.43
1:D:81:ASP:C	1:D:81:ASP:OD1	2.61	0.43
1:E:297:HIS:HB3	1:E:366:PRO:HD2	1.99	0.43
1:F:344:PHE:HB3	1:F:345:PRO:HD2	2.00	0.43
1:H:189:ASP:OD2	1:H:189:ASP:C	2.62	0.43
1:J:28:ASP:HB2	1:J:50:LYS:O	2.17	0.43
1:A:222:PHE:CD1	1:A:286:VAL:HG11	2.54	0.43
1:A:296:LEU:HD13	1:A:296:LEU:HA	1.79	0.43
1:F:55:GLU:HG3	1:F:57:GLY:H	1.82	0.43
1:F:110:ASN:HB2	2:F:773:FAD:C4X	2.49	0.43
1:F:238:ASP:OD1	1:F:238:ASP:C	2.61	0.43
1:G:28:ASP:O	1:G:248:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ASN:O	1:A:392:SER:HB2	2.19	0.43
1:B:376:SER:O	1:B:377:ASP:C	2.61	0.43
1:G:32:VAL:HG13	1:G:217:VAL:HG21	2.01	0.43
1:I:405:LYS:N	1:I:447:PHE:HE2	2.17	0.43
1:J:269:LEU:HD22	1:J:378:SER:HB3	2.01	0.43
1:L:195:HIS:HA	1:L:199:GLU:OE1	2.18	0.43
1:B:51:VAL:HG12	1:B:52:LEU:N	2.32	0.43
1:B:225:ASN:HA	1:B:226:SER:HA	1.69	0.43
1:B:287:LEU:HD22	1:B:480:ILE:HG13	2.01	0.43
1:C:341:PHE:O	1:C:342:ALA:HB3	2.19	0.43
1:C:476:ARG:HA	1:C:484:ARG:HG2	2.00	0.43
1:D:331:PHE:CE2	1:D:333:SER:HB2	2.54	0.43
1:F:31:ILE:HD13	1:F:255:ILE:HD13	1.99	0.43
1:G:161:ALA:HB1	1:G:410:LEU:HD23	2.00	0.43
1:G:196:ALA:HA	1:G:197:SER:HB2	2.01	0.43
1:I:255:ILE:H	1:I:255:ILE:HG12	1.55	0.43
1:B:379:ASP:C	1:B:381[A]:ARG:H	2.25	0.43
1:D:91:SER:C	1:D:93:ASP:N	2.77	0.43
1:E:39:CYS:HB2	1:E:40:PRO:HD3	2.01	0.43
1:J:244:HIS:N	1:J:244:HIS:CD2	2.87	0.43
1:K:99:ARG:HB3	1:K:461:TYR:OH	2.18	0.43
1:L:127:ILE:HD11	1:L:129:TRP:CE3	2.54	0.43
1:D:236:TYR:CZ	1:D:244:HIS:CB	3.02	0.42
1:D:411:LEU:HB3	1:D:430:PHE:CE1	2.54	0.42
1:E:102:VAL:CG1	1:E:108:MET:HB3	2.49	0.42
1:I:471:LEU:CD2	1:I:477:VAL:HG22	2.48	0.42
1:K:263:SER:HB2	1:K:264:PRO:HD3	2.01	0.42
1:L:341:PHE:O	1:L:342:ALA:HB3	2.18	0.42
1:B:137:THR:O	1:B:141:VAL:HG23	2.18	0.42
1:E:328:GLN:HE22	1:E:406:LYS:HB3	1.84	0.42
1:H:113:VAL:HG22	1:H:317:VAL:O	2.19	0.42
1:I:102:VAL:HG11	1:I:108:MET:HB3	2.01	0.42
1:A:59:LEU:HD23	1:A:213:VAL:HG11	1.99	0.42
1:A:472:ASP:OD1	1:A:474:ASP:N	2.46	0.42
1:C:291:TYR:CD1	1:C:469:GLU:HG3	2.54	0.42
1:D:263:SER:O	1:D:264:PRO:C	2.61	0.42
1:E:153:ALA:HB3	1:E:313:GLU:HG2	2.01	0.42
1:F:140:TRP:CZ2	1:F:203:LYS:HB3	2.54	0.42
1:H:274:PRO:HB2	1:H:277:TYR:HB3	2.01	0.42
1:I:21:LEU:HD11	1:I:212:ALA:HB1	2.01	0.42
1:A:137:THR:CG2	1:A:505:MET:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HG23	1:B:214:HIS:HE1	1.80	0.42
1:D:338:ILE:HG23	1:D:339:PRO:HD2	2.01	0.42
1:E:303:PHE:O	1:E:304:ILE:HD13	2.19	0.42
1:G:50:LYS:HD3	1:G:208:ASN:HA	2.01	0.42
1:G:63:TYR:C	1:G:65:ASN:H	2.27	0.42
1:G:72:PHE:HD2	1:G:73:ILE:HD13	1.83	0.42
1:H:475:PHE:CZ	1:H:506:LEU:HD11	2.54	0.42
1:J:8:ASP:OD1	1:J:8:ASP:C	2.61	0.42
1:J:412:SER:OG	1:J:426:GLY:HA2	2.19	0.42
1:K:148:LYS:HA	1:K:149:PRO:HD3	1.92	0.42
1:L:302:ASN:HD21	1:L:391:TYR:HH	1.63	0.42
1:A:404:MET:HE2	1:A:450:PHE:CE2	2.54	0.42
2:B:773:FAD:H9	2:B:773:FAD:H1'1	1.89	0.42
1:D:21:LEU:CD1	1:D:212:ALA:HB1	2.48	0.42
1:E:404:MET:HE2	1:E:450:PHE:HE2	1.85	0.42
1:G:334:LEU:HB3	1:G:335:PRO:HD2	2.02	0.42
1:H:236:TYR:CE1	1:H:244:HIS:HB2	2.53	0.42
1:H:438:PRO:HB2	1:H:447:PHE:CE1	2.54	0.42
1:H:459:TRP:HB3	2:H:773:FAD:C8	2.48	0.42
1:I:27:TYR:O	1:I:248:VAL:HA	2.19	0.42
1:I:303:PHE:HB3	1:I:360:VAL:CG1	2.48	0.42
1:J:275:GLU:HG3	1:J:285:VAL:HG21	2.01	0.42
1:A:116:ARG:HG2	1:A:138:TYR:CD2	2.55	0.42
1:A:459:TRP:HB3	2:A:773:FAD:C8	2.50	0.42
1:D:108:MET:O	1:D:108:MET:HG3	2.20	0.42
1:E:60:PRO:HD3	1:E:103:LEU:HB3	2.01	0.42
1:F:45:LEU:HD23	1:F:45:LEU:HA	1.92	0.42
1:G:268:LEU:HB3	1:G:374:LEU:HD11	2.01	0.42
1:G:297:HIS:HB3	1:G:366:PRO:HD2	2.01	0.42
1:B:138:TYR:HB3	1:B:142:GLU:OE2	2.19	0.42
1:D:162:PHE:CD2	1:D:410:LEU:HD11	2.54	0.42
1:D:255:ILE:CD1	1:D:486:VAL:CG2	2.98	0.42
1:F:258:ALA:O	1:F:262:GLY:HA3	2.20	0.42
1:I:226:SER:HA	1:I:227:SER:HA	1.78	0.42
1:J:250:GLY:O	1:J:251:GLU:HB2	2.19	0.42
1:J:294:GLN:O	1:J:295:PHE:HB2	2.19	0.42
1:K:305:ASN:HB3	1:K:433:LEU:HB3	2.01	0.42
1:B:52:LEU:HA	1:B:210:ARG:O	2.19	0.42
1:B:162:PHE:HB3	1:B:181:THR:OG1	2.19	0.42
1:C:89:PHE:CZ	1:C:97:ASP:HB3	2.54	0.42
1:F:298:ASP:HB2	1:F:388:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:362:LYS:HB2	1:J:458:TYR:CE1	2.55	0.42
1:L:11:TYR:C	1:L:13:SER:H	2.28	0.42
1:L:148:LYS:HA	1:L:149:PRO:HD3	1.93	0.42
1:L:162:PHE:CD2	1:L:410:LEU:HD21	2.55	0.42
1:L:216:SER:O	1:L:236:TYR:HA	2.20	0.42
1:A:29:TYR:HE2	1:A:253:GLU:HG2	1.85	0.42
2:A:773:FAD:H9	2:A:773:FAD:H1'1	1.79	0.42
1:B:153:ALA:HB3	1:B:313:GLU:CD	2.44	0.42
1:F:359:PHE:HZ	1:F:416:LEU:HD11	1.84	0.42
1:H:306:ILE:HG22	1:H:432:ILE:CD1	2.50	0.42
1:I:107:SER:OG	1:I:196:ALA:HB1	2.20	0.42
1:J:220:ILE:HA	1:J:234:VAL:HG12	2.00	0.42
1:J:472:ASP:OD1	1:J:472:ASP:C	2.63	0.42
1:K:440:ASN:C	1:K:442:THR:H	2.28	0.42
1:L:397:LEU:HD21	1:L:452:ARG:NH1	2.35	0.42
1:A:16:TYR:O	1:A:213:VAL:HG22	2.20	0.42
1:A:149:PRO:HB3	1:A:318:THR:HG21	2.01	0.42
1:A:303:PHE:HA	1:A:359:PHE:O	2.20	0.42
1:B:304:ILE:HD11	1:B:437:LEU:HG	2.01	0.42
1:C:56:ARG:HA	1:C:215:ALA:O	2.19	0.42
1:D:35:GLY:HA3	2:D:773:FAD:O5B	2.20	0.42
1:D:304:ILE:HD11	1:D:437:LEU:HG	2.02	0.42
1:F:145:ILE:HG22	1:F:195:HIS:HB3	2.02	0.42
1:G:45:LEU:O	1:G:47:GLU:N	2.53	0.42
1:H:299:ASN:HA	1:H:300:PRO:HD3	1.95	0.42
1:I:1:LEU:HD23	1:I:1:LEU:HA	1.87	0.42
1:I:89:PHE:CZ	1:I:97:ASP:HB3	2.55	0.42
1:J:97:ASP:O	1:J:98:VAL:CG1	2.67	0.42
2:J:773:FAD:H1'1	2:J:773:FAD:H9	1.81	0.42
1:L:238:ASP:OD2	1:L:244:HIS:HE1	2.03	0.42
1:L:298:ASP:HB2	1:L:388:PHE:CE2	2.55	0.42
1:L:307:LEU:HD23	1:L:356:PHE:HB3	2.02	0.42
1:C:389:ASN:HB3	1:C:392:SER:HG	1.85	0.41
1:E:48[A]:LYS:HB2	1:E:48[A]:LYS:HE2	1.83	0.41
1:F:137:THR:CG2	1:F:508:ARG:HB3	2.50	0.41
1:G:230:THR:O	1:G:230:THR:HG22	2.12	0.41
1:G:307:LEU:HD11	1:G:433:LEU:HB2	2.01	0.41
1:I:89:PHE:CE2	1:I:97:ASP:HB3	2.54	0.41
1:J:140:TRP:CD2	1:J:508:ARG:HD2	2.54	0.41
1:L:11:TYR:C	1:L:13:SER:N	2.78	0.41
1:L:205:ASP:OD1	1:L:207:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:HG3	1:B:57:GLY:N	2.35	0.41
1:B:66:LEU:CD1	1:B:108:MET:HE3	2.49	0.41
1:B:99:ARG:HB3	1:B:461:TYR:OH	2.20	0.41
1:B:157:LEU:HD11	1:B:419:TYR:CE1	2.44	0.41
1:C:205:ASP:HA	1:C:206:PRO:HD2	1.74	0.41
1:D:274:PRO:HB2	1:D:277:TYR:HB3	2.02	0.41
1:G:152:GLN:O	1:G:153:ALA:C	2.63	0.41
1:G:265:GLN:HG3	1:G:374:LEU:CD2	2.50	0.41
1:G:299:ASN:ND2	1:G:363:VAL:O	2.51	0.41
1:H:236:TYR:CZ	1:H:244:HIS:CB	3.02	0.41
1:E:200:LEU:HA	1:E:200:LEU:HD23	1.74	0.41
1:F:269:LEU:HD22	1:F:378:SER:HA	2.03	0.41
1:F:327:TYR:CZ	1:F:364:PRO:HB3	2.55	0.41
1:F:506:LEU:O	1:F:510:VAL:HG23	2.20	0.41
1:G:216:SER:O	1:G:236:TYR:HA	2.19	0.41
1:G:244:HIS:CD2	1:G:244:HIS:N	2.88	0.41
1:G:358:HIS:NE2	1:G:360:VAL:HG12	2.34	0.41
1:J:161:ALA:HB2	1:J:416:LEU:HD23	2.02	0.41
1:K:265:GLN:O	1:K:269:LEU:HG	2.20	0.41
1:B:283:ILE:HA	1:B:284:PRO:HD3	1.94	0.41
1:C:330:SER:HA	1:C:358:HIS:O	2.19	0.41
1:C:486:VAL:CG2	1:C:510:VAL:HG11	2.42	0.41
1:G:42:ALA:O	1:G:43:ALA:C	2.62	0.41
1:H:289:HIS:HB3	1:H:292:VAL:HG23	2.01	0.41
1:I:372:ILE:HD13	1:I:384:PRO:HB2	2.00	0.41
1:I:414:ASP:HA	1:I:417:LYS:HG3	2.02	0.41
1:J:301:ARG:CD	1:J:360:VAL:CG1	2.95	0.41
1:J:411:LEU:HB3	1:J:430:PHE:HE1	1.84	0.41
1:K:9:PHE:HB3	1:K:12:LEU:CD1	2.50	0.41
1:K:440:ASN:O	1:K:442:THR:N	2.54	0.41
1:L:130:ASP:O	1:L:134:VAL:HG23	2.20	0.41
1:L:365:GLY:HA2	1:L:493:TYR:HB3	2.01	0.41
1:C:299:ASN:ND2	1:C:363:VAL:O	2.52	0.41
1:C:303:PHE:HA	1:C:359:PHE:O	2.20	0.41
2:C:773:FAD:H9	2:C:773:FAD:H1'1	1.89	0.41
1:D:41:LEU:O	1:D:42:ALA:C	2.63	0.41
1:F:325:ASN:O	1:F:364:PRO:HD2	2.18	0.41
1:G:66:LEU:O	1:G:194:ARG:HD2	2.20	0.41
1:H:114:TYR:CE1	1:H:501:GLY:HA2	2.56	0.41
1:H:412:SER:OG	1:H:426:GLY:HA2	2.21	0.41
1:H:459:TRP:HB3	2:H:773:FAD:C8M	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:PHE:CZ	1:K:328:GLN:HB3	2.53	0.41
1:L:27:TYR:CD2	1:L:52:LEU:HB2	2.55	0.41
1:A:122:PHE:O	1:A:129:TRP:HD1	2.01	0.41
1:A:150:ASP:O	1:A:151:LYS:C	2.64	0.41
1:B:24:GLU:HA	1:B:245:GLN:O	2.20	0.41
1:C:21:LEU:HD11	1:C:212:ALA:HB2	1.94	0.41
1:G:127:ILE:HD11	1:G:129:TRP:CE3	2.53	0.41
1:H:27:TYR:O	1:H:248:VAL:HA	2.21	0.41
1:H:56:ARG:HG2	2:H:773:FAD:C4A	2.51	0.41
2:J:773:FAD:HM71	2:J:773:FAD:HM83	1.89	0.41
1:L:157:LEU:HD13	1:L:419:TYR:OH	2.20	0.41
1:L:326:PHE:CE1	1:L:403:GLY:HA2	2.55	0.41
1:A:101:ARG:HD3	1:A:381:ARG:HH22	1.86	0.41
1:B:299:ASN:OD1	1:B:299:ASN:N	2.54	0.41
1:D:110:ASN:HA	2:D:773:FAD:C6	2.51	0.41
1:F:12:LEU:HD22	1:F:59:LEU:HD13	2.01	0.41
1:G:249:ARG:H	1:G:249:ARG:HG3	1.74	0.41
1:G:358:HIS:CD2	1:G:360:VAL:HG12	2.55	0.41
1:I:157:LEU:HD11	1:I:419:TYR:CZ	2.56	0.41
1:J:110:ASN:O	1:J:194:ARG:NH2	2.48	0.41
1:A:303:PHE:HE1	1:A:305:ASN:HD21	1.69	0.41
1:D:154:TRP:CZ3	1:D:157:LEU:HD22	2.56	0.41
1:E:179:ALA:HA	1:E:322:ILE:HG22	2.03	0.41
1:E:233:GLY:HA3	1:E:246:ALA:O	2.21	0.41
1:F:145:ILE:O	1:F:187:THR:HG22	2.19	0.41
1:F:219:LYS:HD3	1:K:376:SER:OG	2.21	0.41
1:H:344:PHE:HB3	1:H:345:PRO:HD2	2.02	0.41
1:L:40:PRO:HG2	1:L:507:GLY:HA3	2.02	0.41
1:B:114:TYR:CE1	1:B:501:GLY:HA2	2.56	0.41
1:B:231:ALA:HB3	1:B:482:ALA:O	2.20	0.41
1:B:322:ILE:HD13	1:B:322:ILE:HA	1.89	0.41
1:C:30:VAL:O	1:C:255:ILE:HG22	2.21	0.41
1:D:242:THR:HA	1:D:243:PRO:HD3	1.94	0.41
1:E:127:ILE:HD11	1:E:129:TRP:CE2	2.55	0.41
1:F:89:PHE:CZ	1:F:97:ASP:HB3	2.56	0.41
1:F:99:ARG:HD3	1:F:261:ILE:HD13	2.01	0.41
1:F:459:TRP:HB3	2:F:773:FAD:C8M	2.50	0.41
1:H:391:TYR:OH	1:H:400:CYS:SG	2.75	0.41
1:I:197:SER:HG	1:I:504:LEU:HD21	1.84	0.41
1:I:282:ASN:HB2	1:L:284:PRO:HD3	2.03	0.41
1:J:4:THR:HG23	1:J:189:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:376:SER:HA	1:J:377:ASP:CB	2.41	0.41
1:J:458:TYR:O	1:J:459:TRP:HB2	2.20	0.41
1:K:22:GLU:OE1	1:K:210:ARG:NH2	2.54	0.41
1:L:313:GLU:HA	1:L:314:PRO:HD3	1.76	0.41
1:A:383:ALA:HA	1:A:384:PRO:HD2	1.90	0.41
1:B:89:PHE:CE2	1:B:97:ASP:HB3	2.56	0.41
1:C:3:THR:O	1:C:4:THR:C	2.64	0.41
1:D:222:PHE:HB3	1:D:229:VAL:HG12	2.03	0.41
1:D:261:ILE:HG23	1:D:384:PRO:HG2	2.02	0.41
1:E:250:GLY:O	1:E:251:GLU:HB2	2.21	0.41
1:F:218:GLU:OE2	1:F:237:LYS:CD	2.67	0.41
1:J:107:SER:OG	1:J:197:SER:CB	2.68	0.41
1:J:225:ASN:HA	1:J:226:SER:HA	1.80	0.41
1:J:323:THR:HG22	1:J:324:SER:H	1.86	0.41
1:J:327:TYR:CD1	1:J:497:SER:HA	2.56	0.41
1:L:11:TYR:HB2	1:L:14:PHE:CZ	2.56	0.41
1:A:153:ALA:HB3	1:A:313:GLU:OE2	2.20	0.40
1:A:411:LEU:HB3	1:A:430:PHE:CE1	2.56	0.40
1:D:460:HIS:ND1	1:D:499:PRO:HD3	2.36	0.40
2:D:773:FAD:H9	2:D:773:FAD:H1'	1.93	0.40
1:E:106:THR:HB	2:E:773:FAD:O4'	2.21	0.40
1:E:301:ARG:NH2	1:E:343:PHE:O	2.45	0.40
1:F:39:CYS:N	1:F:40:PRO:HD2	2.36	0.40
1:J:513:LYS:HA	1:J:513:LYS:HD2	1.81	0.40
1:K:376:SER:HA	1:K:377:ASP:HA	1.90	0.40
1:C:499:PRO:O	1:C:500:GLN:C	2.63	0.40
1:D:55:GLU:HG2	1:D:103:LEU:HA	2.03	0.40
1:D:293:GLY:CA	1:D:372:ILE:CG2	2.97	0.40
1:E:46:SER:HB3	1:E:209:LEU:HD13	2.02	0.40
1:E:99:ARG:HB3	1:E:461:TYR:OH	2.22	0.40
1:F:182:ARG:O	1:F:319:VAL:HA	2.21	0.40
1:G:315:SER:HB2	1:G:332:SER:OG	2.21	0.40
1:H:21:LEU:HA	1:H:21:LEU:HD23	1.82	0.40
1:I:346:ASN:OD1	1:I:349:TYR:HB2	2.21	0.40
1:I:411:LEU:HB3	1:I:430:PHE:HE1	1.85	0.40
1:J:196:ALA:HB3	1:J:198:ASP:OD1	2.22	0.40
1:K:498:HIS:HA	1:K:499:PRO:HD3	1.99	0.40
1:L:298:ASP:HB2	1:L:388:PHE:CD2	2.56	0.40
1:L:330:SER:HA	1:L:358:HIS:O	2.21	0.40
1:L:471:LEU:HD23	1:L:477:VAL:HA	2.03	0.40
1:A:187:THR:HB	1:A:195:HIS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:O	1:B:127:ILE:HG13	2.22	0.40
1:B:263:SER:O	1:B:264:PRO:C	2.63	0.40
1:C:103:LEU:CD2	1:C:211:VAL:HG11	2.51	0.40
1:I:69:SER:C	1:I:71:GLY:N	2.79	0.40
1:I:238:ASP:OD2	1:I:242:THR:HB	2.22	0.40
1:K:397:LEU:HD21	1:K:448:GLU:HG2	2.03	0.40
1:A:387:LYS:HE3	1:A:389:ASN:OD1	2.21	0.40
1:C:236:TYR:CE1	1:C:244:HIS:HB2	2.56	0.40
1:D:263:SER:HB2	1:D:264:PRO:HD3	2.03	0.40
1:D:274:PRO:HB3	1:F:128:GLU:HB2	2.03	0.40
1:E:147:TYR:CE2	1:E:195:HIS:CD2	3.10	0.40
1:G:201:LEU:HD13	1:G:211:VAL:HG21	2.03	0.40
1:G:450:PHE:O	1:G:454:ALA:HB3	2.22	0.40
1:H:249:ARG:O	1:H:250:GLY:C	2.63	0.40
1:H:513:LYS:HD2	1:H:513:LYS:HA	1.88	0.40
1:I:105:GLY:HA2	2:I:773:FAD:O3B	2.21	0.40
1:I:510:VAL:HG12	1:I:514:ILE:HD11	2.04	0.40
1:J:362:LYS:HB2	1:J:458:TYR:CD1	2.57	0.40
1:A:84:THR:HB	1:A:85:PRO:HD2	2.04	0.40
1:A:296:LEU:HD22	1:A:464:GLY:CA	2.51	0.40
1:B:422:GLU:HG3	1:B:424:LEU:HG	2.04	0.40
1:C:296:LEU:HD22	1:C:464:GLY:CA	2.51	0.40
1:E:103:LEU:HD12	1:E:103:LEU:HA	1.83	0.40
1:E:367:LEU:HD12	1:E:395:THR:HB	2.03	0.40
1:H:19:THR:HG22	1:H:238:ASP:HB2	2.04	0.40
1:H:138:TYR:O	1:H:142:GLU:HG3	2.21	0.40
1:H:427:ILE:HD12	1:H:427:ILE:O	2.21	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	521/521 (100%)	485 (93%)	31 (6%)	5 (1%)	12	41
1	B	521/521 (100%)	474 (91%)	36 (7%)	11 (2%)	5	24
1	C	520/521 (100%)	476 (92%)	39 (8%)	5 (1%)	12	41
1	D	520/521 (100%)	470 (90%)	42 (8%)	8 (2%)	8	32
1	E	520/521 (100%)	482 (93%)	34 (6%)	4 (1%)	16	46
1	F	521/521 (100%)	476 (91%)	37 (7%)	8 (2%)	8	32
1	G	521/521 (100%)	479 (92%)	32 (6%)	10 (2%)	6	27
1	H	521/521 (100%)	485 (93%)	30 (6%)	6 (1%)	10	37
1	I	520/521 (100%)	481 (92%)	33 (6%)	6 (1%)	10	37
1	J	520/521 (100%)	480 (92%)	35 (7%)	5 (1%)	12	41
1	K	521/521 (100%)	466 (89%)	45 (9%)	10 (2%)	6	27
1	L	521/521 (100%)	476 (91%)	38 (7%)	7 (1%)	9	35
All	All	6247/6252 (100%)	5730 (92%)	432 (7%)	85 (1%)	9	33

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	SER
1	B	228	GLY
1	B	229	VAL
1	B	280	SER
1	B	378	SER
1	C	255	ILE
1	D	378	SER
1	E	378	SER
1	E	487	ASP
1	F	253	GLU
1	F	377	ASP
1	F	378	SER
1	G	197	SER
1	G	377	ASP
1	G	378	SER
1	H	394	SER
1	I	253	GLU
1	I	375	ASN
1	J	197	SER
1	J	251	GLU
1	K	107	SER
1	L	197	SER

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Mol	Chain	Res	Type
1	L	379	ASP
1	L	520	ALA
1	A	377	ASP
1	A	487	ASP
1	B	128	GLU
1	B	375	ASN
1	C	124	ALA
1	D	122	PHE
1	F	487	ASP
1	G	46	SER
1	G	123	SER
1	I	378	SER
1	J	377	ASP
1	K	376	SER
1	K	440	ASN
1	K	441	GLN
1	L	250	GLY
1	L	251	GLU
1	L	376	SER
1	B	487	ASP
1	C	197	SER
1	D	280	SER
1	E	253	GLU
1	F	280	SER
1	F	394	SER
1	G	342	ALA
1	J	250	GLY
1	J	295	PHE
1	K	96	ASP
1	K	153	ALA
1	B	4	THR
1	B	102	VAL
1	C	33	GLY
1	D	92	GLY
1	D	102	VAL
1	G	4	THR
1	G	250	GLY
1	H	423	ASP
1	I	167	VAL
1	K	413	SER
1	K	487	ASP
1	L	151	LYS

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Mol	Chain	Res	Type
1	A	378	SER
1	A	423[A]	ASP
1	A	423[B]	ASP
1	D	465	CYS
1	G	196	ALA
1	H	443	ASP
1	H	487	ASP
1	I	274	PRO
1	K	492	PRO
1	C	5	SER
1	D	228	GLY
1	F	119	THR
1	F	254	VAL
1	H	451	CYS
1	B	254	VAL
1	E	254	VAL
1	D	254	VAL
1	G	254	VAL
1	H	102	VAL
1	I	33	GLY
1	K	418	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	442/440 (100%)	412 (93%)	30 (7%)	14	42
1	B	441/440 (100%)	410 (93%)	31 (7%)	14	41
1	C	441/440 (100%)	413 (94%)	28 (6%)	16	45
1	D	441/440 (100%)	405 (92%)	36 (8%)	10	35
1	E	441/440 (100%)	411 (93%)	30 (7%)	14	42
1	F	442/440 (100%)	408 (92%)	34 (8%)	12	37
1	G	442/440 (100%)	406 (92%)	36 (8%)	11	35
1	H	442/440 (100%)	407 (92%)	35 (8%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	441/440 (100%)	413 (94%)	28 (6%)	16	45
1	J	439/440 (100%)	414 (94%)	25 (6%)	18	49
1	K	442/440 (100%)	409 (92%)	33 (8%)	12	38
1	L	442/440 (100%)	400 (90%)	42 (10%)	8	29
All	All	5296/5280 (100%)	4908 (93%)	388 (7%)	13	39

All (388) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	52	LEU
1	A	58	THR
1	A	66	LEU
1	A	121	ILE
1	A	127	ILE
1	A	151	LYS
1	A	157	LEU
1	A	160	THR
1	A	187	THR
1	A	193	THR
1	A	207	ASN
1	A	226	SER
1	A	229	VAL
1	A	242	THR
1	A	253	GLU
1	A	254	VAL
1	A	255	ILE
1	A	280	SER
1	A	296	LEU
1	A	323	THR
1	A	372	ILE
1	A	378	SER
1	A	380	VAL
1	A	381	ARG
1	A	394	SER
1	A	410	LEU
1	A	428	ASP
1	A	469	GLU
1	A	508	ARG
1	B	53	VAL
1	B	65	ASN

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Mol	Chain	Res	Type
1	B	116	ARG
1	B	119	THR
1	B	127	ILE
1	B	183	LEU
1	B	207	ASN
1	B	224	SER
1	B	226	SER
1	B	227	SER
1	B	229	VAL
1	B	253	GLU
1	B	254	VAL
1	B	261	ILE
1	B	289	HIS
1	B	296	LEU
1	B	313	GLU
1	B	316	THR
1	B	323	THR
1	B	348	THR
1	B	371	SER
1	B	372	ILE
1	B	381[A]	ARG
1	B	381[B]	ARG
1	B	394	SER
1	B	407	ILE
1	B	410	LEU
1	B	427	ILE
1	B	469	GLU
1	B	517	GLU
1	B	518	ARG
1	C	1	LEU
1	C	23	LEU
1	C	31	ILE
1	C	58	THR
1	C	65	ASN
1	C	66	LEU
1	C	121	ILE
1	C	127	ILE
1	C	168	LEU
1	C	207	ASN
1	C	221	ILE
1	C	224	SER
1	C	229	VAL

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Mol	Chain	Res	Type
1	C	230	THR
1	C	237	LYS
1	C	254	VAL
1	C	255	ILE
1	C	256	VAL
1	C	289	HIS
1	C	313	GLU
1	C	360	VAL
1	C	372	ILE
1	C	377	ASP
1	C	407	ILE
1	C	417	LYS
1	C	428	ASP
1	C	433	LEU
1	C	518	ARG
1	D	12	LEU
1	D	13	SER
1	D	31	ILE
1	D	90	VAL
1	D	106	THR
1	D	116	ARG
1	D	121	ILE
1	D	123	SER
1	D	127	ILE
1	D	132	ASP
1	D	168	LEU
1	D	197	SER
1	D	221	ILE
1	D	224	SER
1	D	227	SER
1	D	229	VAL
1	D	253	GLU
1	D	254	VAL
1	D	255	ILE
1	D	261	ILE
1	D	276	SER
1	D	281	LEU
1	D	296	LEU
1	D	313	GLU
1	D	314	PRO
1	D	323	THR
1	D	328	GLN

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Mol	Chain	Res	Type
1	D	346	ASN
1	D	368	SER
1	D	371	SER
1	D	381	ARG
1	D	394	SER
1	D	410	LEU
1	D	416	LEU
1	D	427	ILE
1	D	518	ARG
1	E	3	THR
1	E	41	LEU
1	E	53	VAL
1	E	116	ARG
1	E	121	ILE
1	E	151	LYS
1	E	164	GLU
1	E	193	THR
1	E	197	SER
1	E	221	ILE
1	E	229	VAL
1	E	232	ILE
1	E	253	GLU
1	E	254	VAL
1	E	289	HIS
1	E	306	ILE
1	E	323	THR
1	E	360	VAL
1	E	372	ILE
1	E	377	ASP
1	E	378	SER
1	E	385	ASN
1	E	386	VAL
1	E	387	LYS
1	E	407	ILE
1	E	410	LEU
1	E	411	LEU
1	E	422	GLU
1	E	467	VAL
1	E	518	ARG
1	F	6	ASP
1	F	26	SER
1	F	31	ILE

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Mol	Chain	Res	Type
1	F	44	THR
1	F	58	THR
1	F	121	ILE
1	F	127	ILE
1	F	133	LEU
1	F	157	LEU
1	F	171	ASN
1	F	221	ILE
1	F	224	SER
1	F	226	SER
1	F	229	VAL
1	F	251	GLU
1	F	253	GLU
1	F	272	VAL
1	F	276	SER
1	F	289	HIS
1	F	310	ASN
1	F	313	GLU
1	F	338	ILE
1	F	372	ILE
1	F	373	THR
1	F	376	SER
1	F	378	SER
1	F	392	SER
1	F	393	ASN
1	F	421	VAL
1	F	427	ILE
1	F	469	GLU
1	F	494	SER
1	F	516	GLN
1	F	517	GLU
1	G	23	LEU
1	G	65	ASN
1	G	121	ILE
1	G	127	ILE
1	G	151	LYS
1	G	168	LEU
1	G	189	ASP
1	G	207	ASN
1	G	221	ILE
1	G	224	SER
1	G	227	SER

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Mol	Chain	Res	Type
1	G	229	VAL
1	G	230	THR
1	G	242	THR
1	G	248	VAL
1	G	249	ARG
1	G	253	GLU
1	G	254	VAL
1	G	255	ILE
1	G	261	ILE
1	G	280	SER
1	G	288	SER
1	G	289	HIS
1	G	296	LEU
1	G	313	GLU
1	G	316	THR
1	G	323	THR
1	G	353	ASN
1	G	376	SER
1	G	381[A]	ARG
1	G	381[B]	ARG
1	G	386	VAL
1	G	410	LEU
1	G	427	ILE
1	G	469	GLU
1	G	518	ARG
1	H	12	LEU
1	H	37	SER
1	H	66	LEU
1	H	116	ARG
1	H	121	ILE
1	H	127	ILE
1	H	157	LEU
1	H	160	THR
1	H	162	PHE
1	H	168	LEU
1	H	197	SER
1	H	226	SER
1	H	229	VAL
1	H	235	ILE
1	H	242	THR
1	H	281	LEU
1	H	285	VAL

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Mol	Chain	Res	Type
1	H	287	LEU
1	H	289	HIS
1	H	296	LEU
1	H	313	GLU
1	H	355	THR
1	H	360	VAL
1	H	372	ILE
1	H	376	SER
1	H	378	SER
1	H	394	SER
1	H	395	THR
1	H	406	LYS
1	H	410	LEU
1	H	416	LEU
1	H	421	VAL
1	H	427	ILE
1	H	442	THR
1	H	518	ARG
1	I	31	ILE
1	I	58	THR
1	I	66	LEU
1	I	78	GLN
1	I	119	THR
1	I	121	ILE
1	I	136	GLN
1	I	157	LEU
1	I	193	THR
1	I	229	VAL
1	I	248	VAL
1	I	254	VAL
1	I	255	ILE
1	I	277	TYR
1	I	296	LEU
1	I	313	GLU
1	I	320	LEU
1	I	360	VAL
1	I	372	ILE
1	I	373	THR
1	I	378	SER
1	I	380	VAL
1	I	381	ARG
1	I	392	SER

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Mol	Chain	Res	Type
1	I	421	VAL
1	I	427	ILE
1	I	512	SER
1	I	518	ARG
1	J	12	LEU
1	J	24	GLU
1	J	121	ILE
1	J	127	ILE
1	J	151	LYS
1	J	157	LEU
1	J	160	THR
1	J	168	LEU
1	J	178	GLU
1	J	197	SER
1	J	207	ASN
1	J	226	SER
1	J	253	GLU
1	J	287	LEU
1	J	289	HIS
1	J	313	GLU
1	J	353	ASN
1	J	360	VAL
1	J	372	ILE
1	J	381	ARG
1	J	387	LYS
1	J	410	LEU
1	J	421	VAL
1	J	428	ASP
1	J	469	GLU
1	K	3	THR
1	K	10	SER
1	K	93	ASP
1	K	107	SER
1	K	120	LYS
1	K	121	ILE
1	K	123	SER
1	K	127	ILE
1	K	184	THR
1	K	198	ASP
1	K	199	GLU
1	K	205	ASP
1	K	219	LYS

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Mol	Chain	Res	Type
1	K	226	SER
1	K	229	VAL
1	K	249	ARG
1	K	251	GLU
1	K	254	VAL
1	K	276	SER
1	K	282	ASN
1	K	289	HIS
1	K	296	LEU
1	K	307	LEU
1	K	315	SER
1	K	323	THR
1	K	372	ILE
1	K	392	SER
1	K	407	ILE
1	K	421	VAL
1	K	427	ILE
1	K	469	GLU
1	K	497	SER
1	K	518	ARG
1	L	3	THR
1	L	23	LEU
1	L	31	ILE
1	L	53	VAL
1	L	58	THR
1	L	116	ARG
1	L	119	THR
1	L	127	ILE
1	L	156	SER
1	L	160	THR
1	L	168	LEU
1	L	203	LYS
1	L	229	VAL
1	L	239	SER
1	L	244	HIS
1	L	255	ILE
1	L	257	SER
1	L	287	LEU
1	L	289	HIS
1	L	296	LEU
1	L	313	GLU
1	L	316	THR

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Mol	Chain	Res	Type
1	L	338	ILE
1	L	360	VAL
1	L	367	LEU
1	L	371	SER
1	L	372	ILE
1	L	376	SER
1	L	379	ASP
1	L	380	VAL
1	L	394	SER
1	L	401	VAL
1	L	414	ASP
1	L	417	LYS
1	L	424	LEU
1	L	427	ILE
1	L	439	GLU
1	L	442	THR
1	L	458	TYR
1	L	478	THR
1	L	494	SER
1	L	517	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	289	HIS
1	A	299	ASN
1	B	328	GLN
1	B	346	ASN
1	B	361	ASN
1	B	393	ASN
1	C	65	ASN
1	C	75	ASN
1	C	83	GLN
1	C	302	ASN
1	C	310	ASN
1	C	346	ASN
1	C	375	ASN
1	C	441	GLN
1	D	171	ASN
1	D	460	HIS
1	E	245	GLN

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Mol	Chain	Res	Type
1	E	328	GLN
1	E	440	ASN
1	E	441	GLN
1	F	191	ASN
1	F	346	ASN
1	F	516	GLN
1	G	65	ASN
1	G	195	HIS
1	G	294	GLN
1	G	346	ASN
1	G	393	ASN
1	H	65	ASN
1	H	152	GLN
1	H	207	ASN
1	H	302	ASN
1	H	389	ASN
1	I	353	ASN
1	I	385	ASN
1	I	399	HIS
1	J	190	ASN
1	J	325	ASN
1	J	375	ASN
1	J	393	ASN
1	K	155	GLN
1	K	214	HIS
1	K	441	GLN
1	L	177	HIS
1	L	245	GLN
1	L	297	HIS
1	L	310	ASN
1	L	325	ASN
1	L	361	ASN
1	L	393	ASN
1	L	441	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	I	773	-	58,58,58	1.14	6 (10%)	85,89,89	1.73	16 (18%)
2	FAD	E	773	-	58,58,58	1.28	6 (10%)	85,89,89	1.62	22 (25%)
2	FAD	D	773	-	58,58,58	1.15	7 (12%)	85,89,89	1.69	16 (18%)
2	FAD	C	773	-	58,58,58	1.16	5 (8%)	85,89,89	1.67	19 (22%)
2	FAD	J	773	-	58,58,58	1.14	7 (12%)	85,89,89	1.70	20 (23%)
2	FAD	L	773	-	58,58,58	1.23	8 (13%)	85,89,89	1.74	18 (21%)
2	FAD	H	773	-	58,58,58	1.19	5 (8%)	85,89,89	1.71	17 (20%)
2	FAD	G	773	-	58,58,58	1.19	7 (12%)	85,89,89	1.69	20 (23%)
2	FAD	K	773	-	58,58,58	1.07	5 (8%)	85,89,89	1.63	15 (17%)
2	FAD	A	773	-	58,58,58	1.27	7 (12%)	85,89,89	1.54	19 (22%)
2	FAD	F	773	-	58,58,58	1.17	6 (10%)	85,89,89	1.69	16 (18%)
2	FAD	B	773	-	58,58,58	1.25	8 (13%)	85,89,89	1.57	17 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	I	773	-	-	3/34/50/50	0/6/6/6
2	FAD	E	773	-	-	6/34/50/50	0/6/6/6
2	FAD	D	773	-	-	3/34/50/50	0/6/6/6
2	FAD	C	773	-	-	8/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	J	773	-	-	3/34/50/50	0/6/6/6
2	FAD	L	773	-	-	5/34/50/50	0/6/6/6
2	FAD	H	773	-	-	5/34/50/50	0/6/6/6
2	FAD	G	773	-	-	9/34/50/50	0/6/6/6
2	FAD	K	773	-	-	9/34/50/50	0/6/6/6
2	FAD	A	773	-	-	12/34/50/50	0/6/6/6
2	FAD	F	773	-	-	5/34/50/50	0/6/6/6
2	FAD	B	773	-	-	10/34/50/50	0/6/6/6

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	773	FAD	C4X-N5	4.65	1.40	1.30
2	A	773	FAD	C4X-N5	4.13	1.39	1.30
2	C	773	FAD	C4X-N5	3.80	1.39	1.30
2	B	773	FAD	PA-O3P	3.71	1.63	1.59
2	A	773	FAD	PA-O3P	3.70	1.63	1.59
2	F	773	FAD	C4X-N5	3.68	1.38	1.30
2	L	773	FAD	C10-N1	3.67	1.40	1.33
2	I	773	FAD	C4X-N5	3.57	1.38	1.30
2	L	773	FAD	C4X-N5	3.51	1.38	1.30
2	J	773	FAD	C10-N1	3.42	1.40	1.33
2	A	773	FAD	C2A-N1A	3.36	1.39	1.33
2	K	773	FAD	C4X-N5	3.35	1.38	1.30
2	J	773	FAD	C4X-N5	3.34	1.38	1.30
2	E	773	FAD	PA-O3P	3.34	1.63	1.59
2	G	773	FAD	C4X-N5	3.31	1.37	1.30
2	I	773	FAD	C2A-N3A	3.25	1.39	1.33
2	D	773	FAD	C4X-N5	3.24	1.37	1.30
2	G	773	FAD	C10-N1	3.19	1.39	1.33
2	H	773	FAD	C2A-N1A	3.11	1.39	1.33
2	E	773	FAD	C2A-N3A	3.11	1.39	1.33
2	H	773	FAD	C2A-N3A	3.03	1.39	1.33
2	F	773	FAD	C10-N1	2.93	1.39	1.33
2	H	773	FAD	C4X-N5	2.88	1.37	1.30
2	B	773	FAD	C4X-N5	2.85	1.36	1.30
2	F	773	FAD	C2A-N1A	2.83	1.39	1.33
2	E	773	FAD	C2A-N1A	2.82	1.38	1.33
2	C	773	FAD	C10-N1	2.81	1.38	1.33
2	B	773	FAD	C2A-N1A	2.78	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	773	FAD	C10-N1	2.74	1.38	1.33
2	E	773	FAD	C10-N1	2.73	1.38	1.33
2	L	773	FAD	P-O3P	2.72	1.62	1.59
2	D	773	FAD	C2A-N1A	2.71	1.38	1.33
2	D	773	FAD	C8A-N7A	2.71	1.36	1.31
2	H	773	FAD	C8A-N7A	2.68	1.36	1.31
2	K	773	FAD	C2A-N1A	2.68	1.38	1.33
2	I	773	FAD	C2A-N1A	2.66	1.38	1.33
2	D	773	FAD	C2A-N3A	2.65	1.38	1.33
2	G	773	FAD	C2A-N1A	2.65	1.38	1.33
2	A	773	FAD	C10-N1	2.64	1.38	1.33
2	B	773	FAD	P-O3P	2.63	1.62	1.59
2	L	773	FAD	PA-O3P	2.61	1.62	1.59
2	C	773	FAD	C5A-N7A	-2.60	1.34	1.39
2	L	773	FAD	C2A-N3A	2.60	1.38	1.33
2	G	773	FAD	C5'-C4'	2.55	1.55	1.51
2	A	773	FAD	P-O3P	2.55	1.62	1.59
2	B	773	FAD	C8A-N7A	2.53	1.36	1.31
2	K	773	FAD	C2A-N3A	2.51	1.38	1.33
2	L	773	FAD	C2A-N1A	2.47	1.38	1.33
2	B	773	FAD	C10-N1	2.42	1.38	1.33
2	F	773	FAD	C2A-N3A	2.41	1.38	1.33
2	D	773	FAD	PA-O3P	2.39	1.62	1.59
2	K	773	FAD	C8A-N7A	2.39	1.36	1.31
2	G	773	FAD	C8A-N7A	2.36	1.36	1.31
2	J	773	FAD	C2A-N1A	2.36	1.38	1.33
2	B	773	FAD	C5A-N7A	-2.34	1.34	1.39
2	G	773	FAD	C5A-N7A	-2.30	1.34	1.39
2	C	773	FAD	C2A-N1A	2.28	1.38	1.33
2	F	773	FAD	C8A-N7A	2.27	1.36	1.31
2	F	773	FAD	PA-O3P	2.27	1.61	1.59
2	C	773	FAD	C8A-N7A	2.24	1.36	1.31
2	B	773	FAD	C2A-N3A	2.21	1.37	1.33
2	K	773	FAD	C10-N1	2.21	1.37	1.33
2	L	773	FAD	C5A-N7A	-2.19	1.35	1.39
2	D	773	FAD	C5A-N7A	-2.18	1.35	1.39
2	A	773	FAD	C5A-N7A	-2.17	1.35	1.39
2	I	773	FAD	C8A-N7A	2.16	1.35	1.31
2	J	773	FAD	P-O3P	2.13	1.61	1.59
2	J	773	FAD	C2A-N3A	2.12	1.37	1.33
2	L	773	FAD	C8A-N7A	2.11	1.35	1.31
2	J	773	FAD	C5A-N7A	-2.11	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	773	FAD	O4B-C4B	-2.10	1.40	1.45
2	J	773	FAD	C8A-N7A	2.06	1.35	1.31
2	G	773	FAD	C2A-N3A	2.05	1.37	1.33
2	I	773	FAD	C10-N1	2.05	1.37	1.33
2	E	773	FAD	C8A-N7A	2.04	1.35	1.31
2	I	773	FAD	C5A-N7A	-2.02	1.35	1.39
2	H	773	FAD	C4X-C10	-2.01	1.38	1.44

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	773	FAD	N3A-C2A-N1A	-6.23	119.15	128.58
2	F	773	FAD	N3A-C2A-N1A	-6.03	119.46	128.58
2	I	773	FAD	C5A-C4A-N3A	-5.78	118.75	126.72
2	J	773	FAD	N3A-C2A-N1A	-5.75	119.87	128.58
2	D	773	FAD	N3A-C2A-N1A	-5.68	119.98	128.58
2	G	773	FAD	N3A-C2A-N1A	-5.53	120.21	128.58
2	L	773	FAD	N3A-C2A-N1A	-5.50	120.25	128.58
2	L	773	FAD	C5A-C4A-N3A	-5.16	119.62	126.72
2	I	773	FAD	N3A-C2A-N1A	-5.04	120.95	128.58
2	E	773	FAD	C5A-C4A-N3A	-4.93	119.92	126.72
2	A	773	FAD	N3A-C2A-N1A	-4.88	121.19	128.58
2	H	773	FAD	C5A-C4A-N3A	-4.84	120.06	126.72
2	B	773	FAD	C5A-C4A-N3A	-4.83	120.06	126.72
2	K	773	FAD	C5A-C4A-N3A	-4.80	120.11	126.72
2	B	773	FAD	N3A-C2A-N1A	-4.56	121.67	128.58
2	C	773	FAD	C5A-C4A-N3A	-4.48	120.55	126.72
2	F	773	FAD	C5A-C4A-N3A	-4.41	120.64	126.72
2	H	773	FAD	N3A-C2A-N1A	-4.41	121.90	128.58
2	K	773	FAD	N3A-C2A-N1A	-4.39	121.94	128.58
2	E	773	FAD	N3A-C2A-N1A	-4.32	122.04	128.58
2	G	773	FAD	C5A-C4A-N3A	-4.30	120.80	126.72
2	D	773	FAD	C5A-C4A-N3A	-4.24	120.88	126.72
2	J	773	FAD	N9A-C8A-N7A	-4.23	107.93	113.94
2	F	773	FAD	N9A-C8A-N7A	-4.18	108.01	113.94
2	H	773	FAD	C4X-C10-N10	4.13	122.40	116.48
2	D	773	FAD	N9A-C8A-N7A	-4.09	108.13	113.94
2	J	773	FAD	C5A-C4A-N3A	-4.01	121.20	126.72
2	G	773	FAD	N9A-C8A-N7A	-3.99	108.28	113.94
2	K	773	FAD	C5A-N7A-C8A	3.98	109.71	103.45
2	L	773	FAD	N9A-C8A-N7A	-3.94	108.35	113.94
2	G	773	FAD	C5A-N7A-C8A	3.89	109.56	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	773	FAD	N9A-C8A-N7A	-3.88	108.42	113.94
2	K	773	FAD	C4A-C5A-N7A	-3.86	106.17	110.58
2	L	773	FAD	C5A-N7A-C8A	3.85	109.50	103.45
2	D	773	FAD	C5A-N7A-C8A	3.83	109.48	103.45
2	A	773	FAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	I	773	FAD	N3A-C4A-N9A	3.78	133.60	127.17
2	C	773	FAD	C5A-N7A-C8A	3.77	109.37	103.45
2	I	773	FAD	C5A-N7A-C8A	3.76	109.36	103.45
2	F	773	FAD	C4-N3-C2	-3.73	119.03	125.64
2	I	773	FAD	C4-N3-C2	-3.73	119.03	125.64
2	C	773	FAD	N9A-C8A-N7A	-3.70	108.69	113.94
2	B	773	FAD	C5A-N7A-C8A	3.68	109.24	103.45
2	B	773	FAD	N9A-C8A-N7A	-3.68	108.71	113.94
2	I	773	FAD	C2A-N3A-C4A	3.67	120.80	111.83
2	F	773	FAD	C5A-N7A-C8A	3.67	109.22	103.45
2	L	773	FAD	C2A-N3A-C4A	3.61	120.65	111.83
2	F	773	FAD	C2A-N3A-C4A	3.57	120.56	111.83
2	G	773	FAD	C4A-C5A-N7A	-3.56	106.51	110.58
2	C	773	FAD	C2A-N3A-C4A	3.56	120.52	111.83
2	D	773	FAD	C4-N3-C2	-3.54	119.35	125.64
2	H	773	FAD	C10-C4X-N5	-3.48	117.71	124.81
2	D	773	FAD	O4-C4-C4X	-3.44	117.44	126.53
2	J	773	FAD	C5A-N7A-C8A	3.44	108.86	103.45
2	I	773	FAD	N9A-C8A-N7A	-3.43	109.07	113.94
2	D	773	FAD	O2A-PA-O3P	3.43	116.53	107.27
2	G	773	FAD	C4X-C10-N10	3.38	121.32	116.48
2	D	773	FAD	O4B-C1B-N9A	3.37	114.56	108.09
2	H	773	FAD	N3A-C4A-N9A	3.34	132.85	127.17
2	K	773	FAD	O4B-C1B-N9A	3.31	114.45	108.09
2	G	773	FAD	C2A-N3A-C4A	3.29	119.86	111.83
2	L	773	FAD	C10-C4X-N5	-3.27	118.12	124.81
2	H	773	FAD	N9A-C8A-N7A	-3.27	109.30	113.94
2	E	773	FAD	N9A-C8A-N7A	-3.25	109.32	113.94
2	D	773	FAD	C4A-C5A-N7A	-3.25	106.86	110.58
2	L	773	FAD	C4-N3-C2	-3.24	119.88	125.64
2	L	773	FAD	N3A-C4A-N9A	3.20	132.61	127.17
2	H	773	FAD	C5A-N7A-C8A	3.20	108.47	103.45
2	J	773	FAD	C2A-N3A-C4A	3.19	119.62	111.83
2	H	773	FAD	O2-C2-N1	-3.17	116.53	121.80
2	L	773	FAD	C4X-C4-N3	3.16	121.29	113.25
2	B	773	FAD	C4-N3-C2	-3.15	120.04	125.64
2	G	773	FAD	C4-C4X-N5	3.13	122.54	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	773	FAD	C5A-N7A-C8A	3.13	108.37	103.45
2	B	773	FAD	C4A-C5A-N7A	-3.12	107.01	110.58
2	A	773	FAD	C5A-C4A-N3A	-3.12	122.42	126.72
2	E	773	FAD	N3A-C4A-N9A	3.09	132.42	127.17
2	C	773	FAD	C4A-C5A-N7A	-3.08	107.06	110.58
2	L	773	FAD	C4A-C5A-N7A	-3.07	107.07	110.58
2	J	773	FAD	C4-N3-C2	-3.07	120.18	125.64
2	D	773	FAD	C2A-N3A-C4A	3.05	119.29	111.83
2	E	773	FAD	C2A-N3A-C4A	3.05	119.28	111.83
2	A	773	FAD	C5A-N7A-C8A	3.05	108.24	103.45
2	L	773	FAD	C4X-C10-N1	-3.04	117.14	124.59
2	A	773	FAD	C5X-C9A-N10	3.03	120.71	117.97
2	A	773	FAD	C4-N3-C2	-3.01	120.29	125.64
2	H	773	FAD	C4-C4X-N5	3.01	122.37	118.21
2	B	773	FAD	C2A-N3A-C4A	3.01	119.18	111.83
2	K	773	FAD	C2A-N3A-C4A	3.00	119.15	111.83
2	G	773	FAD	C4-N3-C2	-2.99	120.33	125.64
2	G	773	FAD	C4X-C4-N3	2.99	120.86	113.25
2	E	773	FAD	C5X-C9A-N10	2.95	120.63	117.97
2	L	773	FAD	O4B-C1B-N9A	2.94	113.75	108.09
2	H	773	FAD	O2P-P-O3P	2.93	115.20	107.27
2	F	773	FAD	C4X-C4-N3	2.93	120.71	113.25
2	E	773	FAD	O3B-C3B-C4B	-2.92	102.69	111.08
2	I	773	FAD	C4A-C5A-N7A	-2.90	107.26	110.58
2	F	773	FAD	N3A-C4A-N9A	2.90	132.10	127.17
2	H	773	FAD	C4-N3-C2	-2.89	120.52	125.64
2	B	773	FAD	C6A-C5A-C4A	2.82	121.03	117.18
2	G	773	FAD	C10-C4X-N5	-2.81	119.07	124.81
2	D	773	FAD	C4X-C4-N3	2.81	120.40	113.25
2	I	773	FAD	C5X-C9A-N10	2.80	120.50	117.97
2	I	773	FAD	O4-C4-C4X	-2.80	119.14	126.53
2	L	773	FAD	C4X-C10-N10	2.79	120.48	116.48
2	I	773	FAD	O2-C2-N1	-2.79	117.16	121.80
2	J	773	FAD	O3B-C3B-C4B	-2.78	103.10	111.08
2	C	773	FAD	C4X-C4-N3	2.77	120.31	113.25
2	C	773	FAD	O4-C4-C4X	-2.77	119.21	126.53
2	J	773	FAD	O4B-C1B-N9A	2.76	113.39	108.09
2	I	773	FAD	C9A-C5X-N5	-2.75	119.53	122.45
2	H	773	FAD	C6A-C5A-C4A	2.75	120.93	117.18
2	G	773	FAD	C10-N1-C2	2.74	122.79	116.85
2	I	773	FAD	C4X-C10-N10	2.73	120.39	116.48
2	B	773	FAD	C4X-C4-N3	2.72	120.19	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	773	FAD	C4-N3-C2	-2.72	120.82	125.64
2	K	773	FAD	C4X-C10-N10	2.71	120.36	116.48
2	H	773	FAD	C2A-N3A-C4A	2.70	118.43	111.83
2	J	773	FAD	O5'-C5'-C4'	-2.69	102.17	109.36
2	F	773	FAD	O2A-PA-O3P	2.69	114.55	107.27
2	G	773	FAD	O2-C2-N3	2.68	123.72	118.58
2	B	773	FAD	N3A-C4A-N9A	2.67	131.71	127.17
2	I	773	FAD	C6A-C5A-C4A	2.66	120.81	117.18
2	G	773	FAD	O4-C4-C4X	-2.65	119.53	126.53
2	C	773	FAD	C4-N3-C2	-2.65	120.94	125.64
2	E	773	FAD	C2B-C1B-N9A	-2.63	106.77	113.30
2	K	773	FAD	C4-N3-C2	-2.63	120.97	125.64
2	L	773	FAD	C4-C4X-N5	2.61	121.82	118.21
2	L	773	FAD	C10-N1-C2	2.61	122.50	116.85
2	F	773	FAD	C10-C4X-N5	-2.61	119.48	124.81
2	H	773	FAD	O2-C2-N3	2.60	123.57	118.58
2	K	773	FAD	C6A-C5A-C4A	2.59	120.72	117.18
2	K	773	FAD	C5A-C4A-N9A	2.56	108.60	105.81
2	B	773	FAD	O4-C4-C4X	-2.55	119.80	126.53
2	J	773	FAD	O4-C4-C4X	-2.54	119.81	126.53
2	J	773	FAD	C10-C4X-N5	-2.54	119.62	124.81
2	F	773	FAD	C4X-C10-N1	-2.53	118.39	124.59
2	B	773	FAD	C4X-C10-N1	-2.52	118.41	124.59
2	J	773	FAD	C4X-C4-N3	2.51	119.65	113.25
2	A	773	FAD	C2A-N3A-C4A	2.51	117.97	111.83
2	E	773	FAD	C4A-C5A-N7A	-2.50	107.72	110.58
2	G	773	FAD	C5A-C4A-N9A	2.50	108.54	105.81
2	L	773	FAD	C5X-N5-C4X	2.50	122.14	118.09
2	E	773	FAD	C10-C4X-N5	-2.50	119.70	124.81
2	J	773	FAD	N3A-C4A-N9A	2.48	131.39	127.17
2	A	773	FAD	C9A-C5X-N5	-2.48	119.82	122.45
2	A	773	FAD	O4-C4-C4X	-2.47	120.01	126.53
2	D	773	FAD	C4X-C10-N10	2.45	119.99	116.48
2	K	773	FAD	C4X-C4-N3	2.45	119.48	113.25
2	J	773	FAD	C4X-C10-N1	-2.43	118.63	124.59
2	E	773	FAD	C6A-C5A-C4A	2.43	120.50	117.18
2	K	773	FAD	N3A-C4A-N9A	2.43	131.29	127.17
2	H	773	FAD	O3B-C3B-C4B	-2.42	104.12	111.08
2	E	773	FAD	O4B-C1B-N9A	2.39	112.67	108.09
2	F	773	FAD	O4-C4-C4X	-2.38	120.24	126.53
2	C	773	FAD	N3A-C4A-N9A	2.38	131.21	127.17
2	C	773	FAD	C9A-C5X-N5	-2.38	119.93	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	773	FAD	O2A-PA-O3P	2.38	113.69	107.27
2	B	773	FAD	O4'-C4'-C5'	-2.37	104.75	109.99
2	A	773	FAD	C4X-C4-N3	2.37	119.30	113.25
2	F	773	FAD	C4A-C5A-N7A	-2.37	107.87	110.58
2	C	773	FAD	C4X-C10-N10	2.37	119.87	116.48
2	E	773	FAD	C9-C9A-N10	-2.36	118.68	121.85
2	G	773	FAD	O3P-P-O1P	-2.36	103.60	110.70
2	E	773	FAD	C4-C4X-N5	2.36	121.46	118.21
2	C	773	FAD	O2P-P-O3P	2.36	113.64	107.27
2	C	773	FAD	C5X-C9A-N10	2.35	120.10	117.97
2	G	773	FAD	C6A-C5A-C4A	2.35	120.38	117.18
2	J	773	FAD	C4A-C5A-N7A	-2.34	107.91	110.58
2	B	773	FAD	C4X-C10-N10	2.33	119.81	116.48
2	C	773	FAD	C10-N1-C2	2.32	121.88	116.85
2	A	773	FAD	N3A-C4A-N9A	2.32	131.12	127.17
2	H	773	FAD	C4A-C5A-N7A	-2.30	107.95	110.58
2	E	773	FAD	O4-C4-C4X	-2.30	120.46	126.53
2	F	773	FAD	C4X-C10-N10	2.30	119.77	116.48
2	C	773	FAD	O2A-PA-O3P	2.29	113.45	107.27
2	B	773	FAD	C4-C4X-C10	2.28	120.85	116.93
2	I	773	FAD	C4X-C4-N3	2.27	119.03	113.25
2	K	773	FAD	O4-C4-C4X	-2.26	120.57	126.53
2	D	773	FAD	N3A-C4A-N9A	2.26	131.01	127.17
2	J	773	FAD	C4-C4X-C10	2.25	120.80	116.93
2	A	773	FAD	C4A-N9A-C8A	2.25	108.10	105.74
2	G	773	FAD	O2-C2-N1	-2.25	118.07	121.80
2	C	773	FAD	C4X-C10-N1	-2.25	119.08	124.59
2	C	773	FAD	C5A-C4A-N9A	2.23	108.24	105.81
2	B	773	FAD	C5A-C4A-N9A	2.22	108.23	105.81
2	I	773	FAD	C10-C4X-N5	-2.21	120.29	124.81
2	K	773	FAD	C10-C4X-N5	-2.18	120.36	124.81
2	F	773	FAD	C9A-C5X-N5	-2.18	120.15	122.45
2	J	773	FAD	O2P-P-O3P	2.16	113.11	107.27
2	C	773	FAD	O4B-C1B-N9A	2.16	112.23	108.09
2	E	773	FAD	O2-C2-N1	-2.16	118.22	121.80
2	E	773	FAD	C4X-C4-N3	2.14	118.71	113.25
2	E	773	FAD	C4X-C10-N10	2.14	119.55	116.48
2	D	773	FAD	C4X-C10-N1	-2.14	119.34	124.59
2	A	773	FAD	C4X-C10-N10	2.13	119.53	116.48
2	D	773	FAD	C5A-C4A-N9A	2.11	108.11	105.81
2	G	773	FAD	C4X-C10-N1	-2.11	119.42	124.59
2	J	773	FAD	C5A-C6A-N6A	-2.11	118.06	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	773	FAD	C5X-C9A-N10	2.11	119.87	117.97
2	A	773	FAD	C10-C4X-N5	-2.10	120.52	124.81
2	L	773	FAD	C5'-C4'-C3'	-2.09	108.27	112.22
2	A	773	FAD	C4-C4X-C10	2.09	120.52	116.93
2	E	773	FAD	O2A-PA-O3P	2.09	112.92	107.27
2	L	773	FAD	C6A-C5A-C4A	2.08	120.02	117.18
2	B	773	FAD	C6-C5X-C9A	2.08	121.91	119.05
2	A	773	FAD	C4X-C10-N1	-2.08	119.49	124.59
2	E	773	FAD	O4B-C4B-C5B	2.06	115.95	109.33
2	A	773	FAD	C7M-C7-C8	2.06	124.96	120.76
2	G	773	FAD	N3A-C4A-N9A	2.05	130.66	127.17
2	J	773	FAD	C4A-N9A-C8A	2.05	107.89	105.74
2	H	773	FAD	O4'-C4'-C5'	-2.04	105.49	109.99
2	A	773	FAD	C8M-C8-C9	-2.03	116.00	119.57
2	J	773	FAD	C4X-C10-N10	2.03	119.39	116.48
2	F	773	FAD	O2'-C2'-C3'	2.01	113.95	109.25

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	773	FAD	N10-C1'-C2'-O2'
2	A	773	FAD	C3'-C4'-C5'-O5'
2	A	773	FAD	O4'-C4'-C5'-O5'
2	A	773	FAD	PA-O3P-P-O5'
2	B	773	FAD	N10-C1'-C2'-O2'
2	B	773	FAD	O4'-C4'-C5'-O5'
2	B	773	FAD	C5'-O5'-P-O1P
2	C	773	FAD	C5B-O5B-PA-O1A
2	C	773	FAD	N10-C1'-C2'-O2'
2	C	773	FAD	N10-C1'-C2'-C3'
2	E	773	FAD	C5'-O5'-P-O1P
2	G	773	FAD	O4'-C4'-C5'-O5'
2	G	773	FAD	C5'-O5'-P-O1P
2	K	773	FAD	C5B-O5B-PA-O1A
2	K	773	FAD	O4'-C4'-C5'-O5'
2	K	773	FAD	O4B-C4B-C5B-O5B
2	K	773	FAD	C3B-C4B-C5B-O5B
2	H	773	FAD	O4'-C4'-C5'-O5'
2	A	773	FAD	O4B-C4B-C5B-O5B
2	C	773	FAD	O4B-C4B-C5B-O5B
2	E	773	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	F	773	FAD	O4B-C4B-C5B-O5B
2	J	773	FAD	O4B-C4B-C5B-O5B
2	L	773	FAD	O4B-C4B-C5B-O5B
2	A	773	FAD	C3B-C4B-C5B-O5B
2	C	773	FAD	C3B-C4B-C5B-O5B
2	E	773	FAD	C3B-C4B-C5B-O5B
2	F	773	FAD	C3B-C4B-C5B-O5B
2	L	773	FAD	C3B-C4B-C5B-O5B
2	B	773	FAD	C3'-C4'-C5'-O5'
2	D	773	FAD	O4B-C4B-C5B-O5B
2	H	773	FAD	O4B-C4B-C5B-O5B
2	A	773	FAD	O3'-C3'-C4'-C5'
2	G	773	FAD	P-O3P-PA-O1A
2	A	773	FAD	O3'-C3'-C4'-O4'
2	D	773	FAD	C3B-C4B-C5B-O5B
2	I	773	FAD	O4B-C4B-C5B-O5B
2	J	773	FAD	C3B-C4B-C5B-O5B
2	G	773	FAD	PA-O3P-P-O5'
2	H	773	FAD	C3B-C4B-C5B-O5B
2	B	773	FAD	P-O3P-PA-O1A
2	A	773	FAD	C2'-C3'-C4'-O4'
2	E	773	FAD	N10-C1'-C2'-O2'
2	F	773	FAD	N10-C1'-C2'-O2'
2	K	773	FAD	N10-C1'-C2'-O2'
2	B	773	FAD	C5'-O5'-P-O2P
2	B	773	FAD	C5'-O5'-P-O3P
2	C	773	FAD	C5B-O5B-PA-O2A
2	E	773	FAD	C2'-C1'-N10-C10
2	G	773	FAD	C5'-O5'-P-O2P
2	G	773	FAD	C5'-O5'-P-O3P
2	I	773	FAD	C2'-C1'-N10-C10
2	K	773	FAD	C5B-O5B-PA-O2A
2	K	773	FAD	C5B-O5B-PA-O3P
2	A	773	FAD	C2'-C3'-C4'-C5'
2	A	773	FAD	P-O3P-PA-O2A
2	G	773	FAD	P-O3P-PA-O2A
2	B	773	FAD	PA-O3P-P-O5'
2	E	773	FAD	C4B-C5B-O5B-PA
2	F	773	FAD	O4'-C4'-C5'-O5'
2	I	773	FAD	C3B-C4B-C5B-O5B
2	C	773	FAD	O3'-C3'-C4'-O4'
2	L	773	FAD	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
2	K	773	FAD	C4B-C5B-O5B-PA
2	G	773	FAD	C3'-C4'-C5'-O5'
2	H	773	FAD	C3'-C4'-C5'-O5'
2	B	773	FAD	P-O3P-PA-O2A
2	F	773	FAD	P-O3P-PA-O1A
2	L	773	FAD	O2'-C2'-C3'-O3'
2	B	773	FAD	O4B-C4B-C5B-O5B
2	G	773	FAD	C2B-C1B-N9A-C8A
2	H	773	FAD	C2B-C1B-N9A-C8A
2	D	773	FAD	N10-C1'-C2'-O2'
2	L	773	FAD	C4B-C5B-O5B-PA
2	K	773	FAD	C2B-C1B-N9A-C8A
2	C	773	FAD	C4B-C5B-O5B-PA
2	A	773	FAD	P-O3P-PA-O1A
2	J	773	FAD	P-O3P-PA-O1A

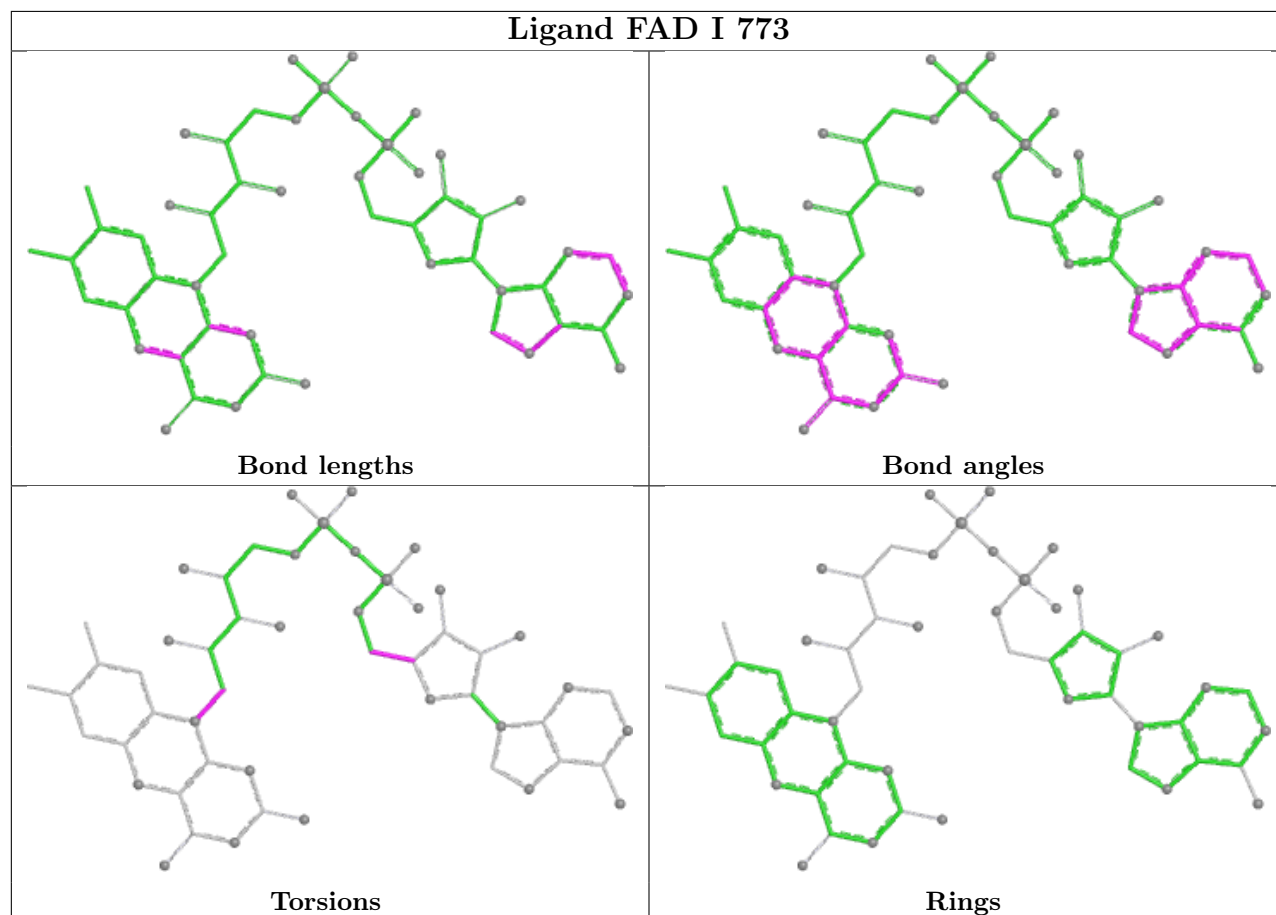
There are no ring outliers.

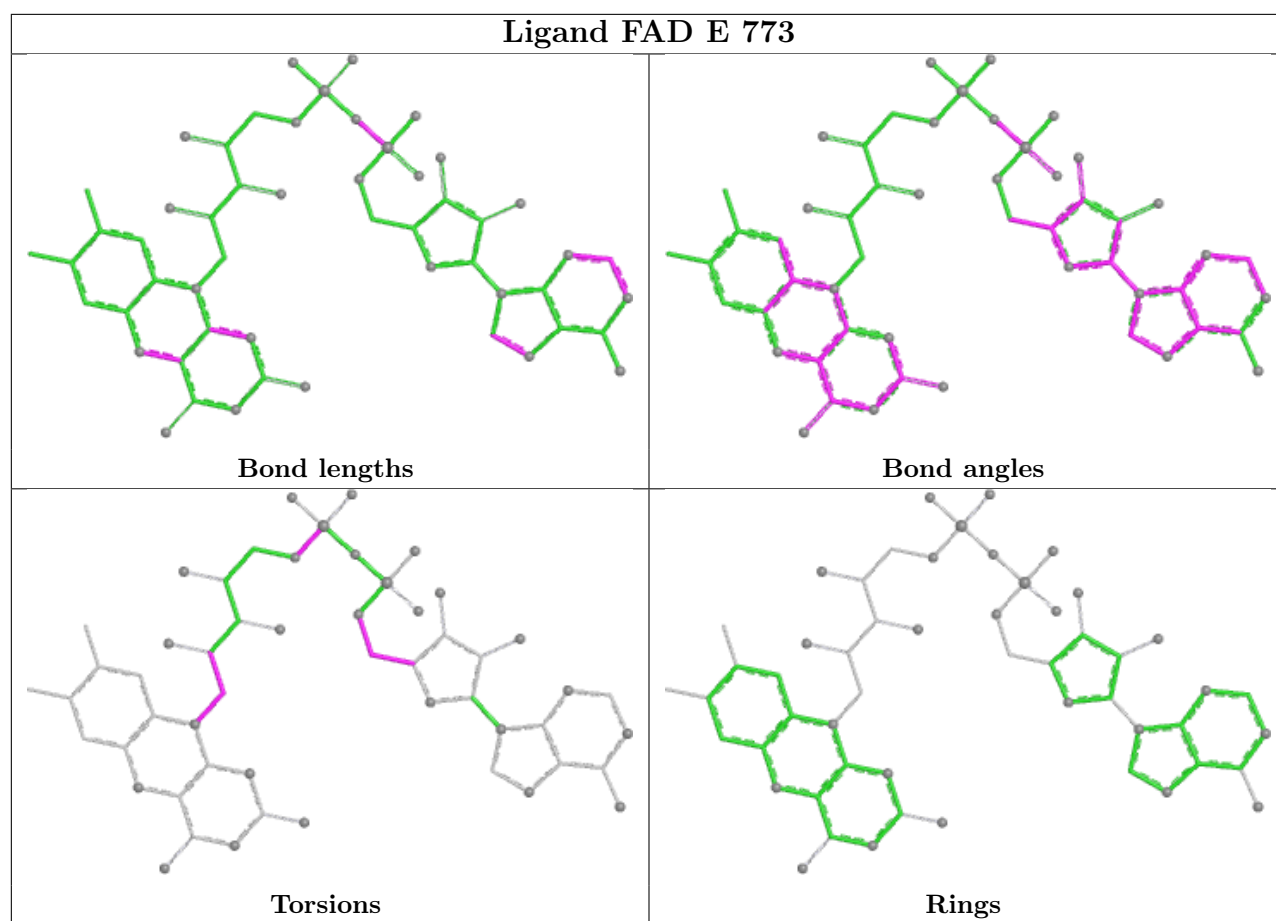
12 monomers are involved in 72 short contacts:

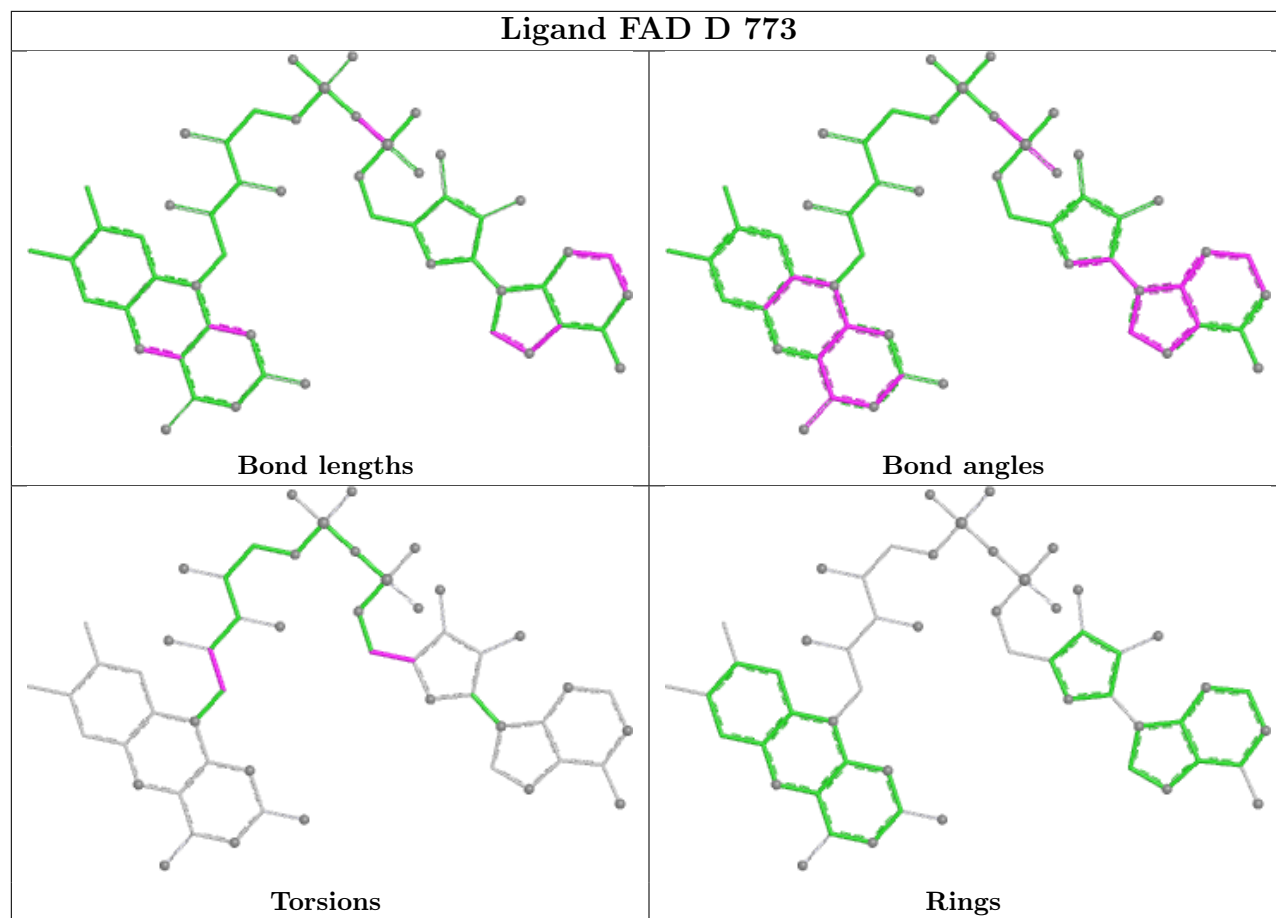
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	773	FAD	5	0
2	E	773	FAD	6	0
2	D	773	FAD	12	0
2	C	773	FAD	6	0
2	J	773	FAD	7	0
2	L	773	FAD	5	0
2	H	773	FAD	7	0
2	G	773	FAD	4	0
2	K	773	FAD	6	0
2	A	773	FAD	5	0
2	F	773	FAD	5	0
2	B	773	FAD	4	0

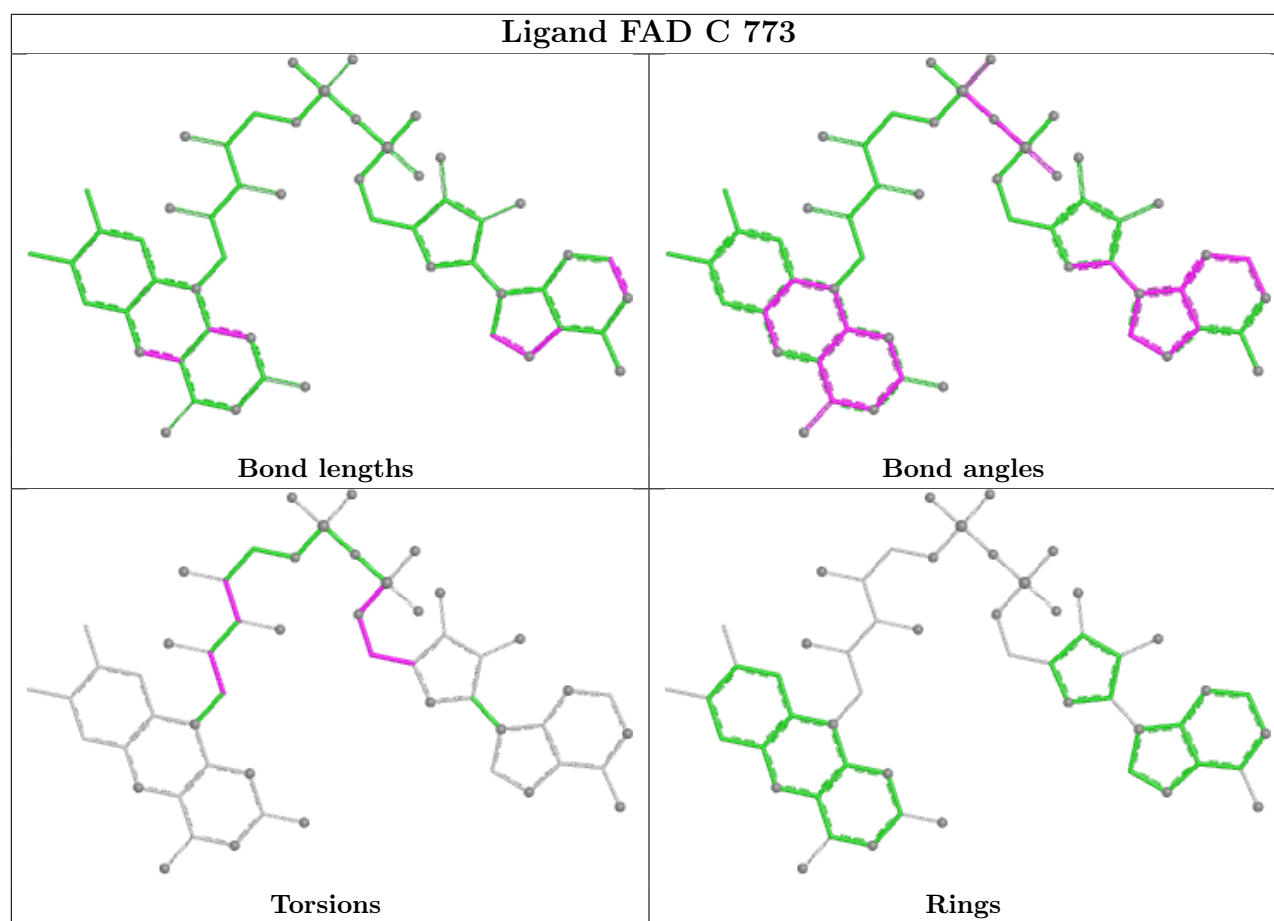
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

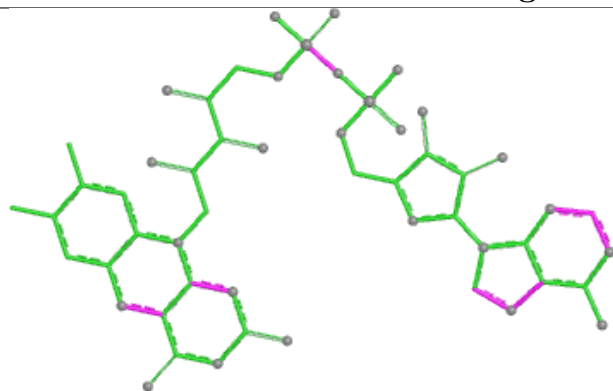




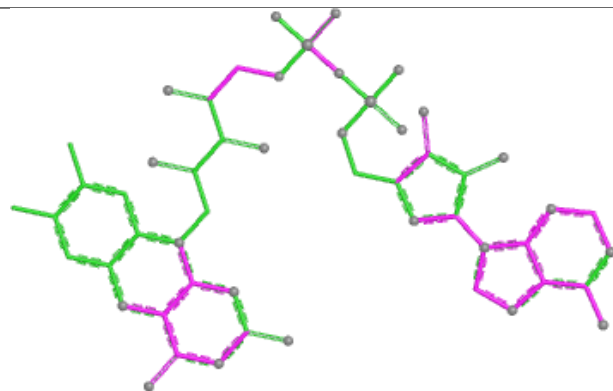




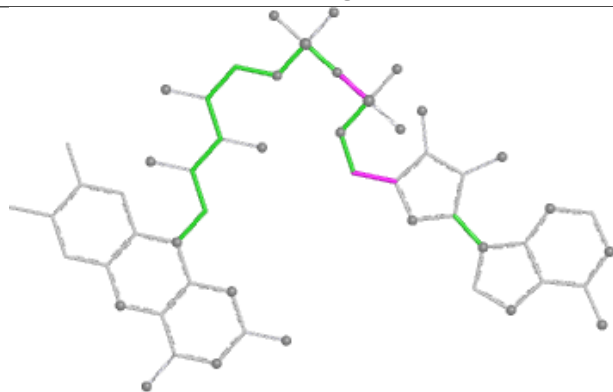
Ligand FAD J 773



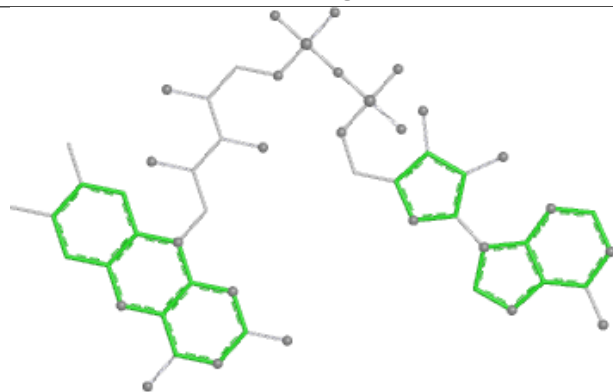
Bond lengths



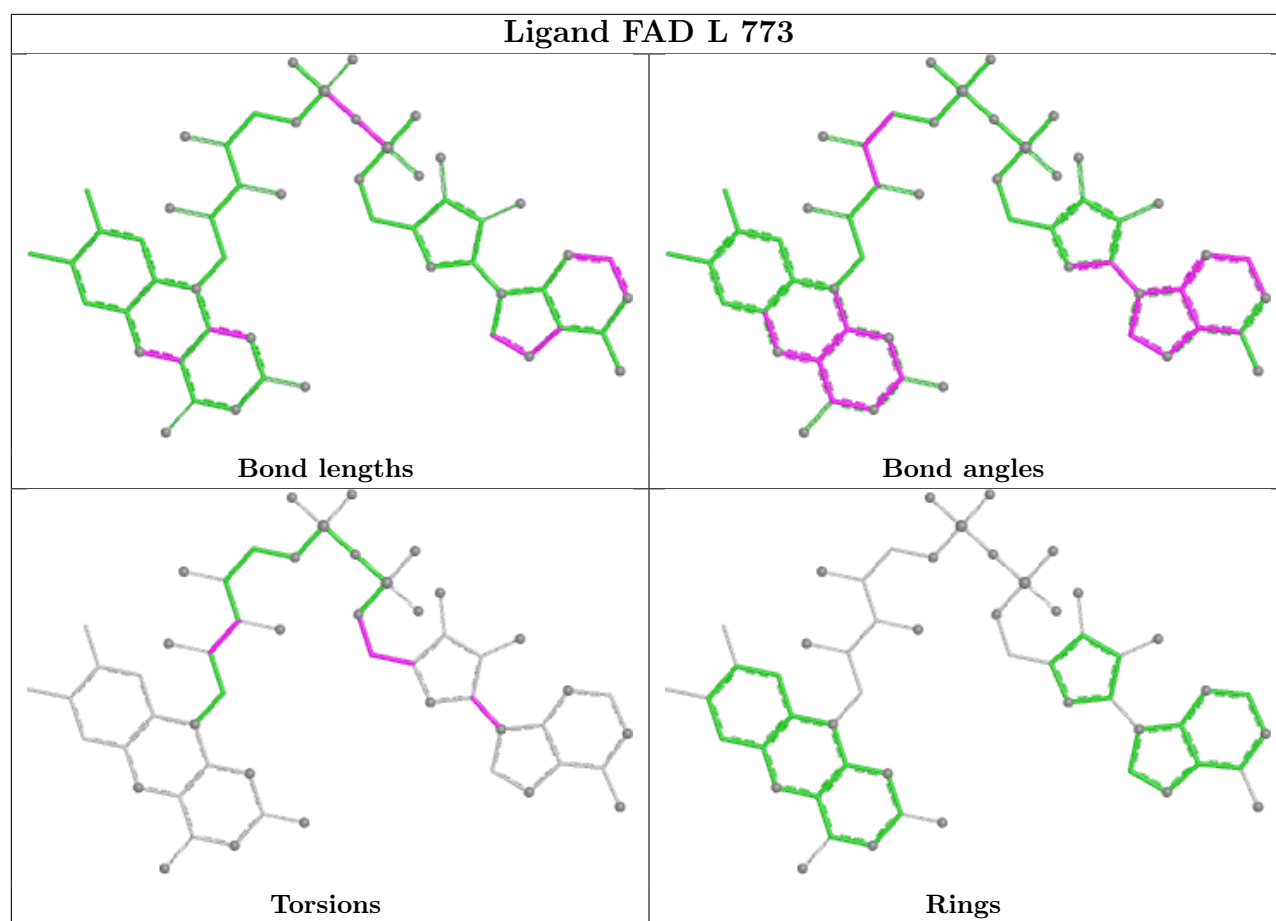
Bond angles

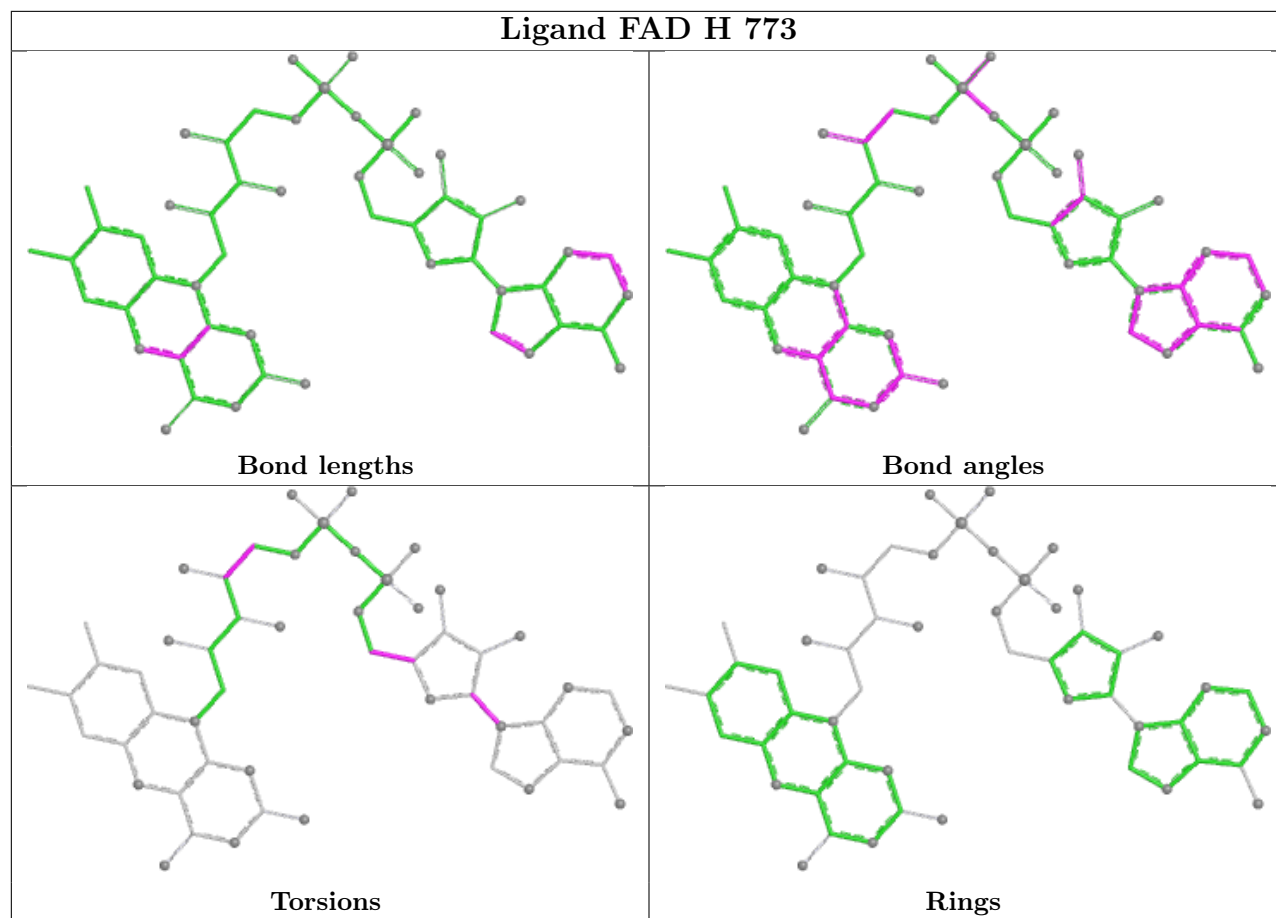


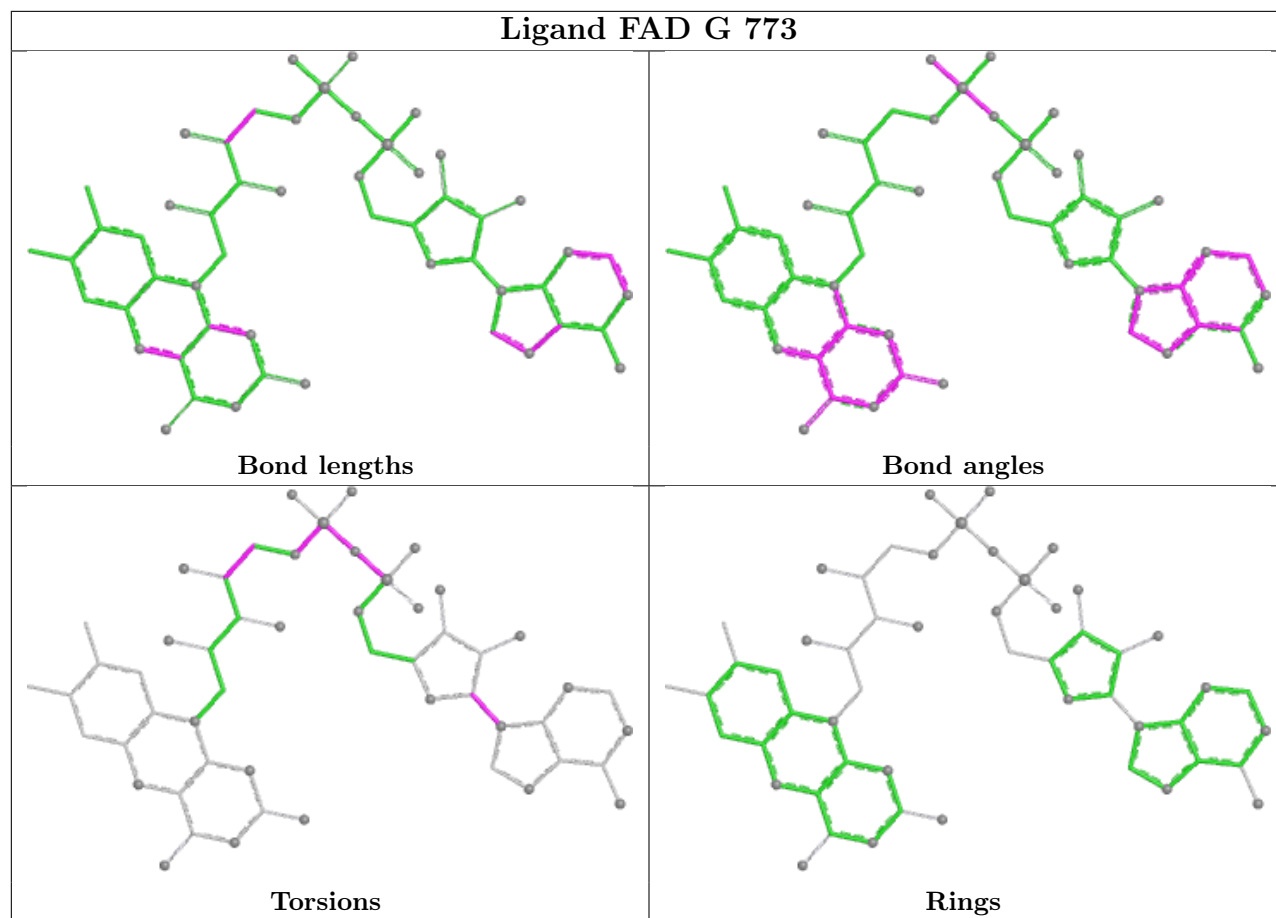
Torsions

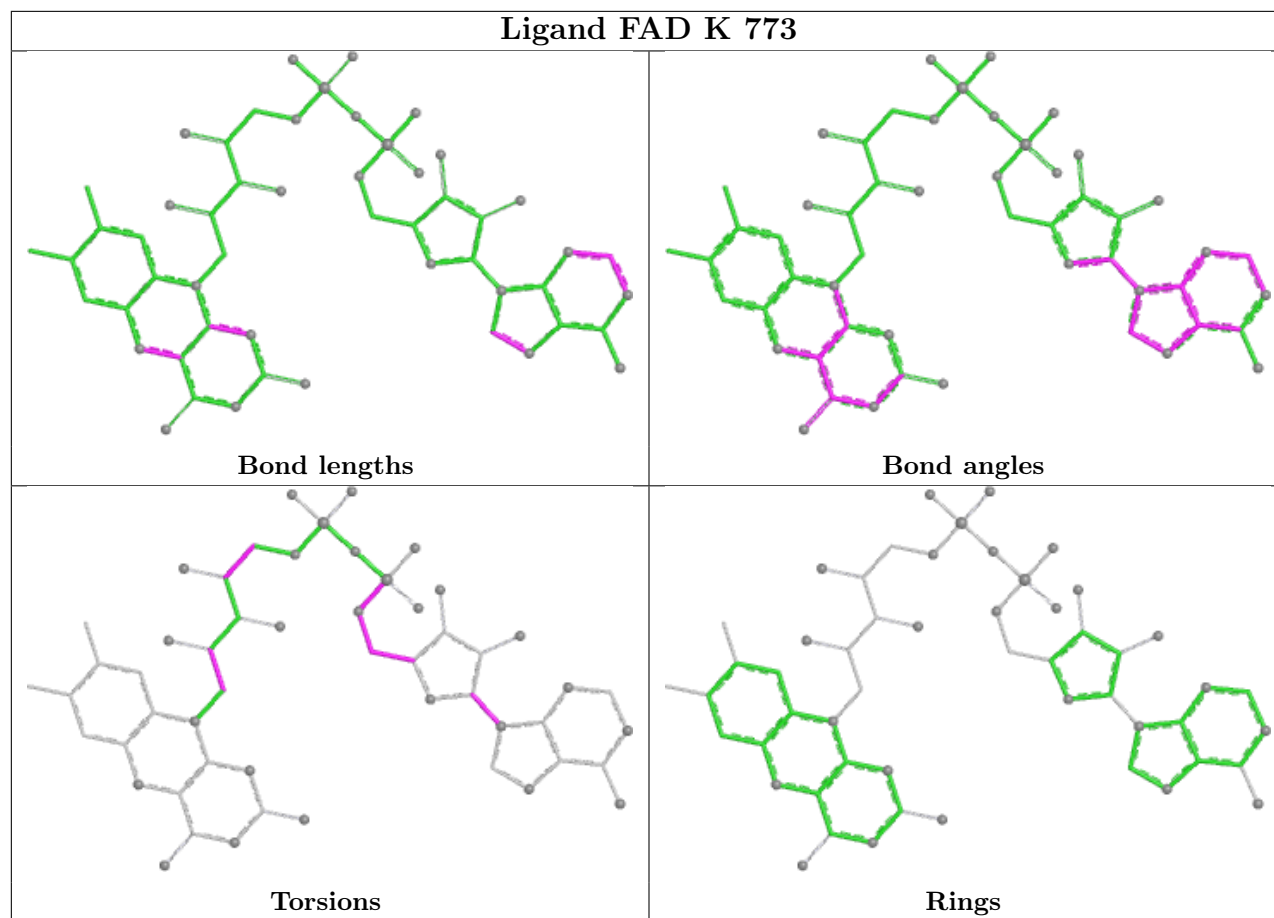


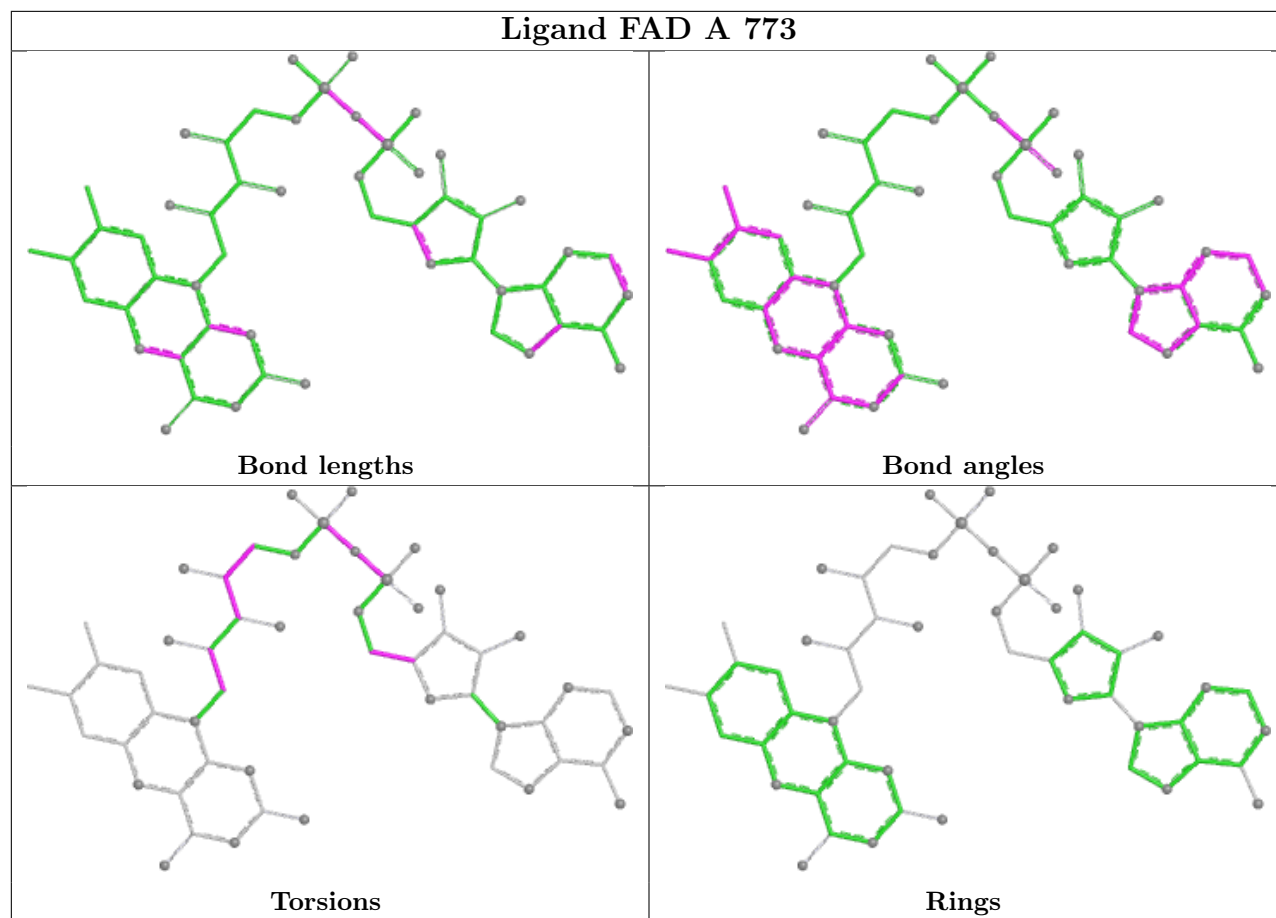
Rings



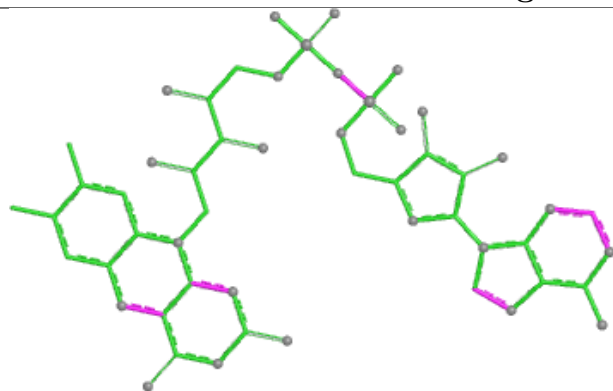




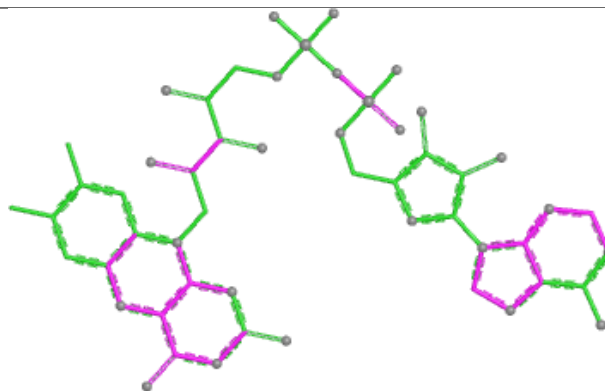




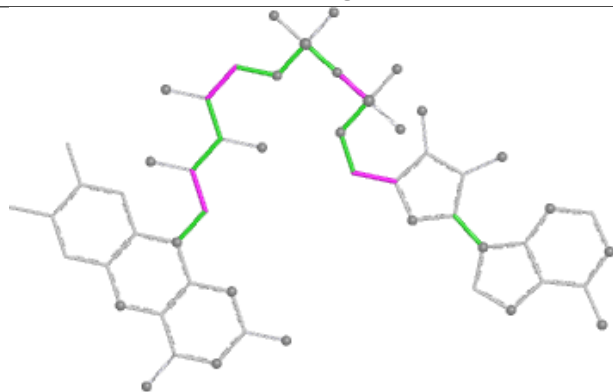
Ligand FAD F 773



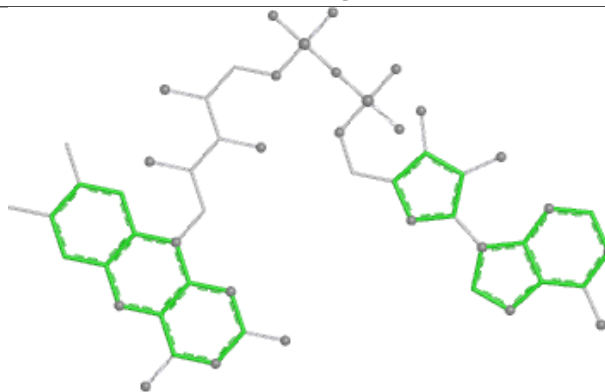
Bond lengths



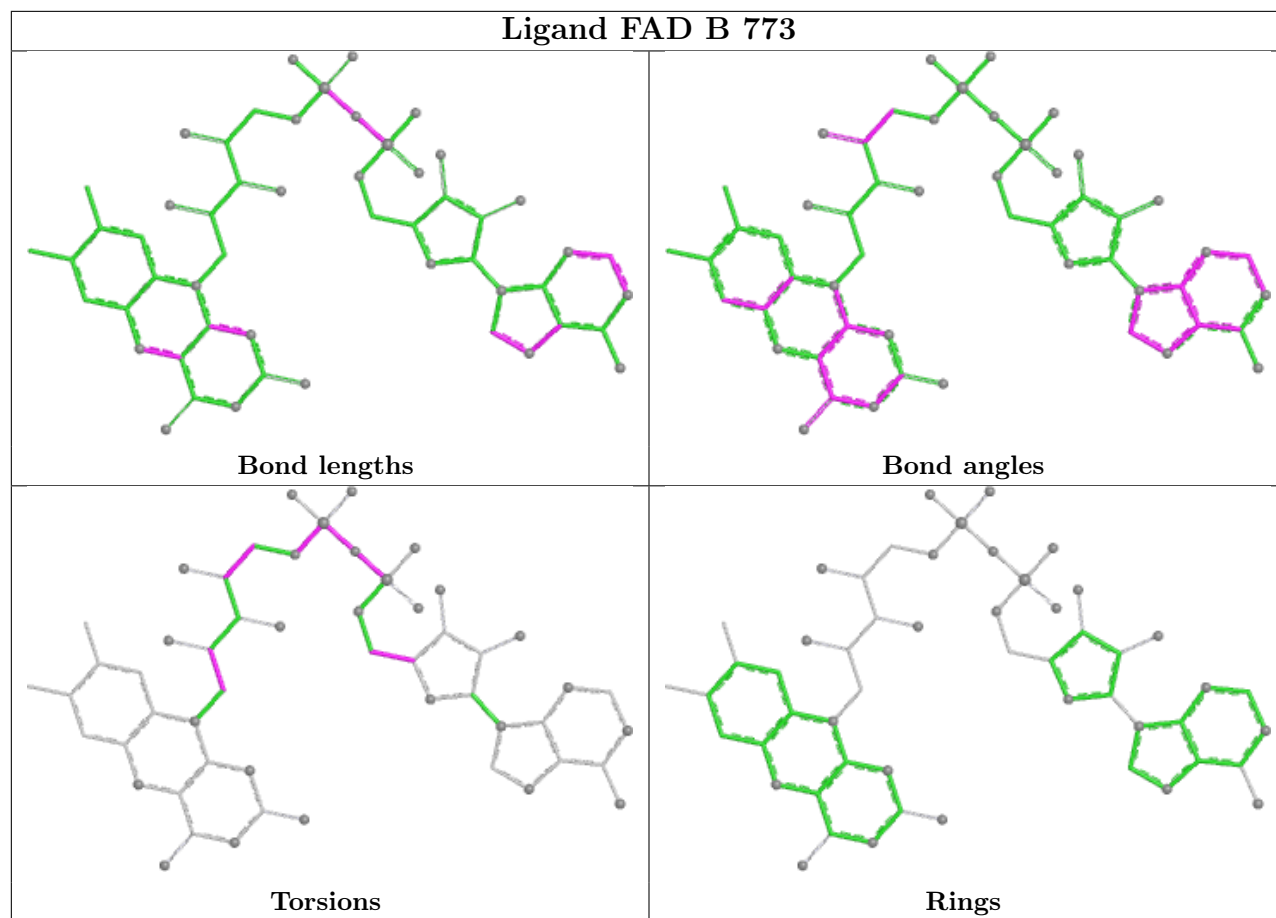
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	521/521 (100%)	-0.54	6 (1%) 76 54	9, 23, 38, 51	2 (0%)
1	B	521/521 (100%)	-0.54	4 (0%) 82 63	12, 23, 35, 53	2 (0%)
1	C	521/521 (100%)	-0.52	3 (0%) 85 69	10, 24, 37, 53	1 (0%)
1	D	521/521 (100%)	-0.52	5 (0%) 79 58	9, 23, 40, 53	1 (0%)
1	E	521/521 (100%)	-0.53	3 (0%) 85 69	10, 25, 39, 50	1 (0%)
1	F	521/521 (100%)	-0.53	4 (0%) 82 63	11, 23, 38, 51	2 (0%)
1	G	521/521 (100%)	-0.57	1 (0%) 91 83	12, 24, 37, 51	2 (0%)
1	H	521/521 (100%)	-0.49	5 (0%) 79 58	12, 26, 41, 50	2 (0%)
1	I	521/521 (100%)	-0.45	4 (0%) 82 63	12, 28, 44, 55	1 (0%)
1	J	521/521 (100%)	-0.46	3 (0%) 85 69	15, 28, 42, 54	1 (0%)
1	K	521/521 (100%)	-0.36	6 (1%) 76 54	13, 31, 46, 57	2 (0%)
1	L	521/521 (100%)	-0.27	1 (0%) 91 83	14, 35, 49, 55	2 (0%)
All	All	6252/6252 (100%)	-0.48	45 (0%) 84 66	9, 26, 43, 57	19 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	226	SER	4.1
1	I	225	ASN	3.9
1	K	226	SER	3.8
1	G	227	SER	3.7
1	A	227	SER	3.6
1	C	225	ASN	3.6
1	D	228	GLY	3.6
1	C	378	SER	3.5
1	D	227	SER	3.4
1	F	225	ASN	3.4
1	K	378	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	227	SER	3.3
1	A	520	ALA	3.1
1	E	227	SER	3.1
1	F	226	SER	3.0
1	C	227	SER	3.0
1	L	228	GLY	3.0
1	K	426	GLY	2.8
1	B	226	SER	2.8
1	I	378	SER	2.8
1	B	227	SER	2.8
1	B	376	SER	2.7
1	D	378	SER	2.7
1	E	228	GLY	2.6
1	H	225	ASN	2.6
1	K	126	GLY	2.5
1	H	227	SER	2.4
1	F	128	GLU	2.4
1	H	226	SER	2.4
1	A	228	GLY	2.4
1	H	519	SER	2.4
1	B	346	ASN	2.3
1	K	153	ALA	2.2
1	E	225	ASN	2.2
1	I	346	ASN	2.2
1	H	378	SER	2.2
1	D	229	VAL	2.1
1	A	519	SER	2.1
1	J	378	SER	2.1
1	A	128	GLU	2.1
1	K	225	ASN	2.1
1	D	225	ASN	2.1
1	A	521	ALA	2.1
1	J	228	GLY	2.0
1	F	520	ALA	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

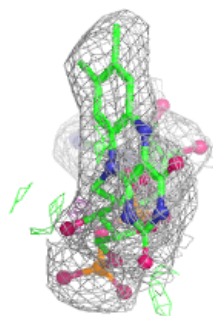
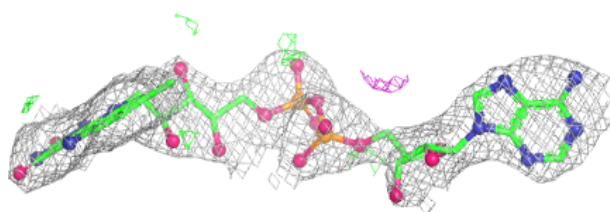
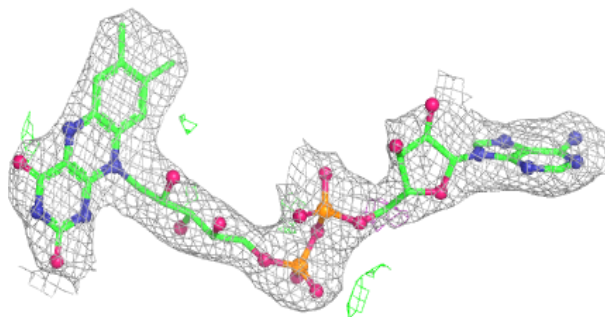
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	FAD	L	773	53/53	0.95	0.07	15,22,26,27	0
2	FAD	J	773	53/53	0.96	0.07	15,18,21,22	0
2	FAD	C	773	53/53	0.97	0.06	7,13,17,19	0
2	FAD	D	773	53/53	0.97	0.06	7,9,11,13	0
2	FAD	E	773	53/53	0.97	0.07	9,14,17,18	0
2	FAD	F	773	53/53	0.97	0.06	7,15,20,22	0
2	FAD	G	773	53/53	0.97	0.06	5,12,14,15	0
2	FAD	H	773	53/53	0.97	0.06	3,11,14,17	0
2	FAD	I	773	53/53	0.97	0.06	11,14,18,20	0
2	FAD	A	773	53/53	0.97	0.06	7,11,13,15	0
2	FAD	K	773	53/53	0.97	0.06	11,17,20,21	0
2	FAD	B	773	53/53	0.97	0.06	6,11,16,17	0

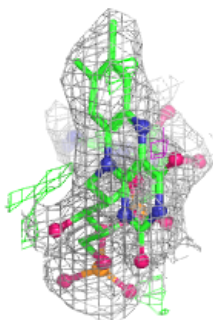
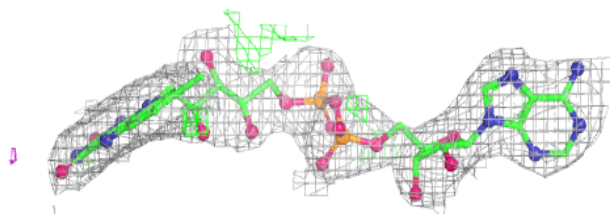
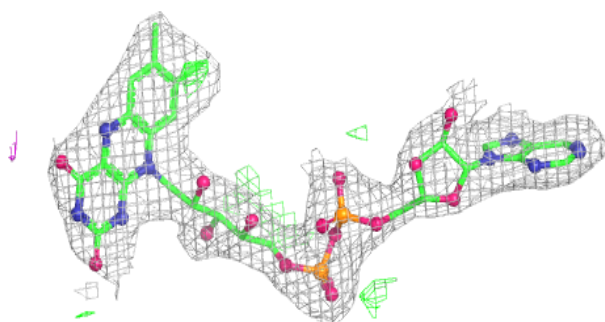
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD L 773:

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

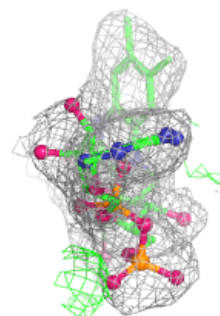
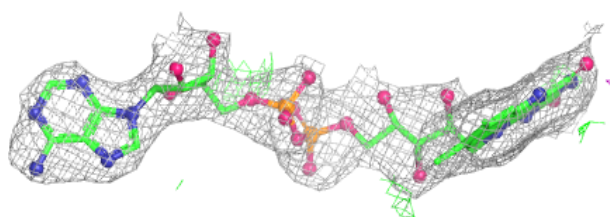
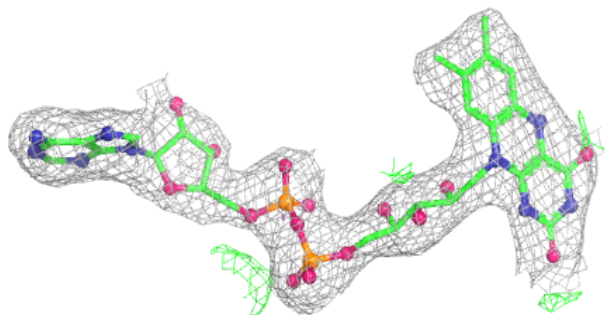
**Electron density around FAD J 773:**

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

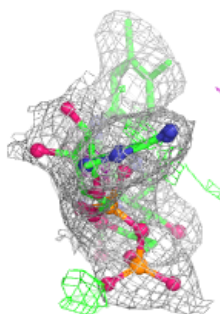
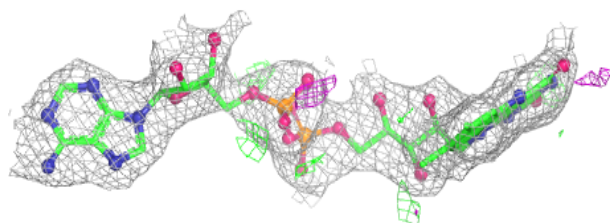
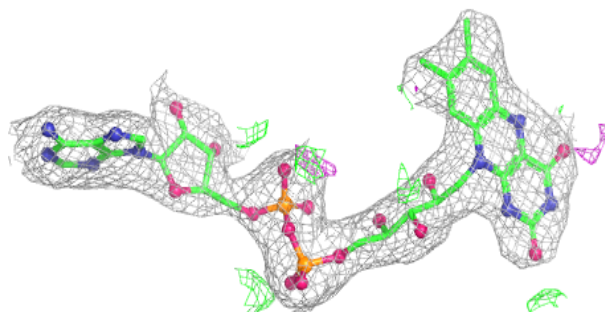


Electron density around FAD C 773:

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

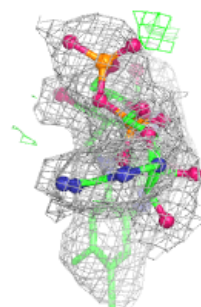
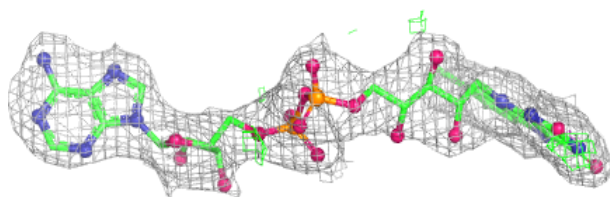
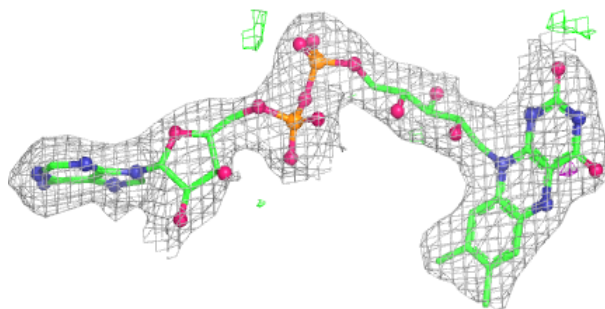
**Electron density around FAD D 773:**

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

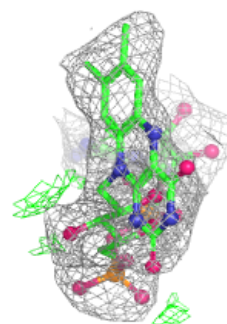
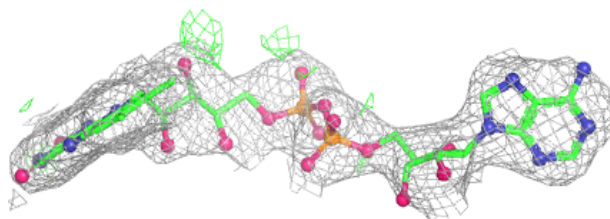
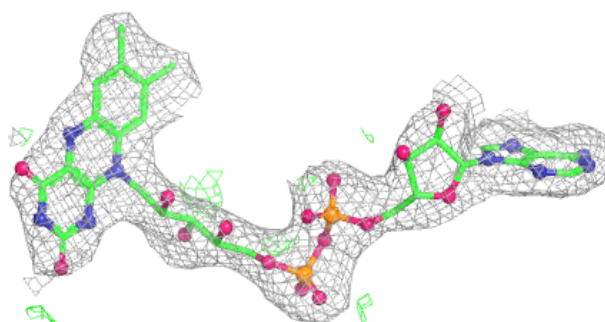


Electron density around FAD E 773:

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

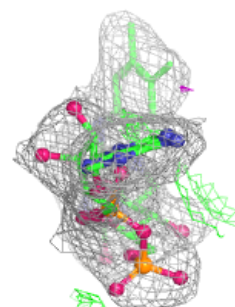
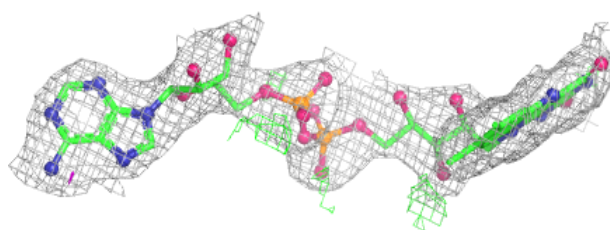
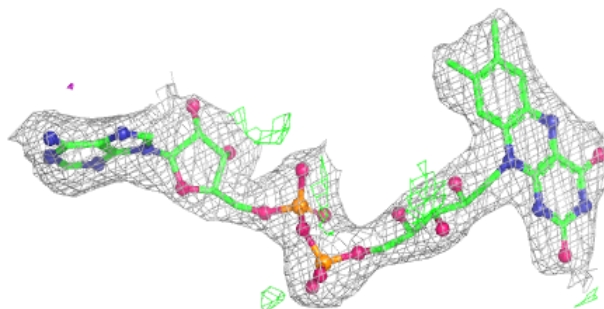
**Electron density around FAD F 773:**

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

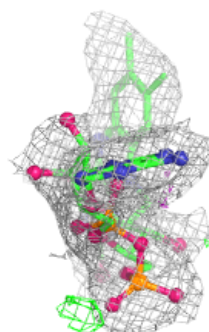
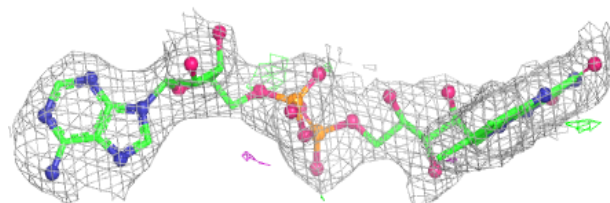
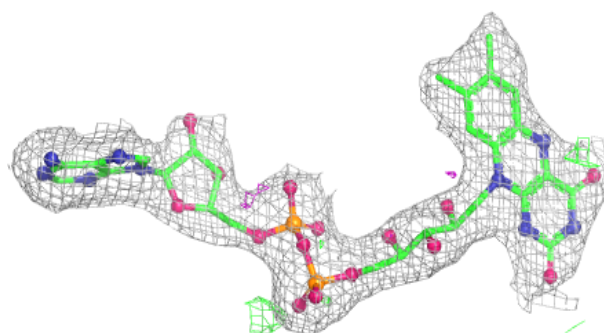


Electron density around FAD G 773:

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

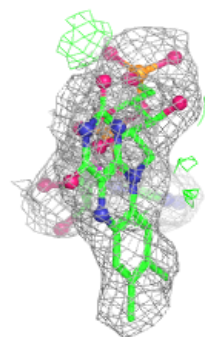
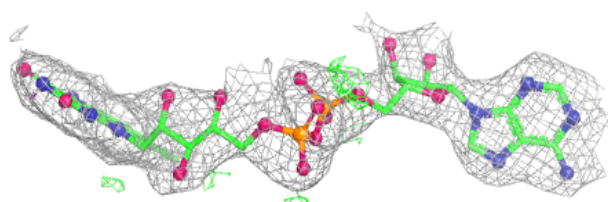
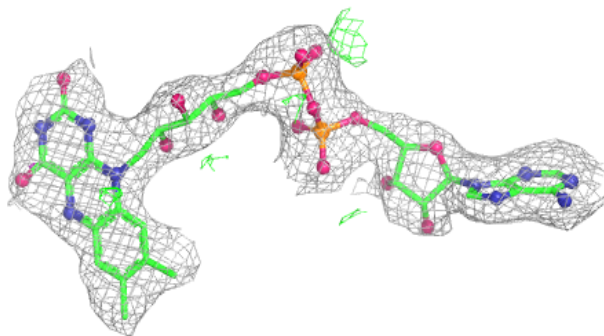
**Electron density around FAD H 773:**

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

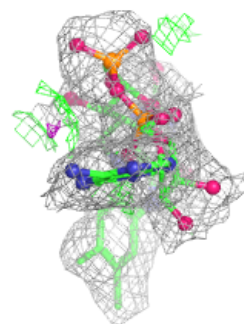
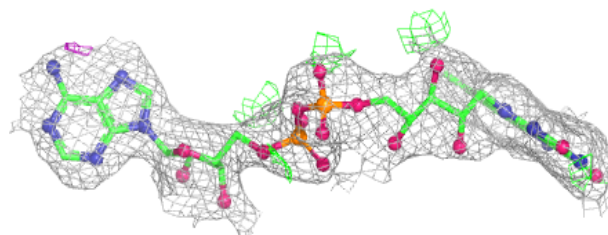
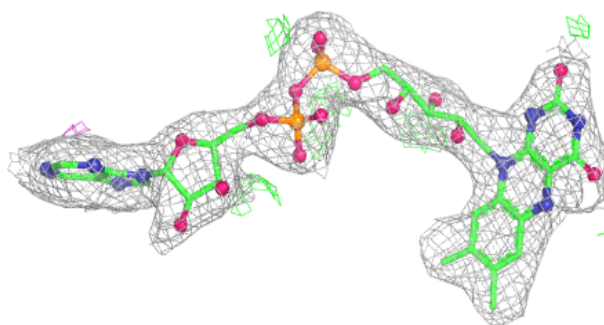


Electron density around FAD I 773:

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

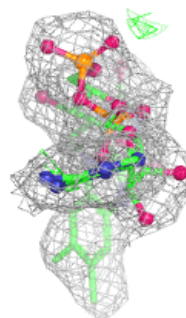
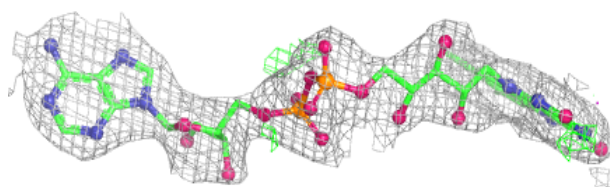
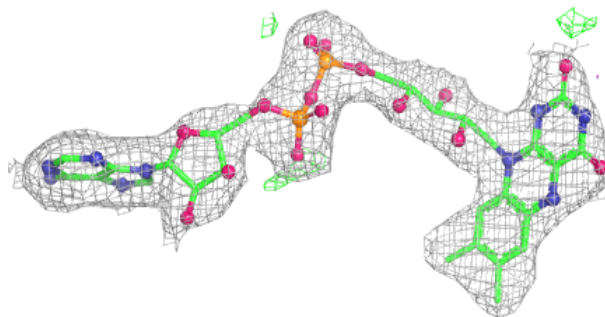
**Electron density around FAD A 773:**

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

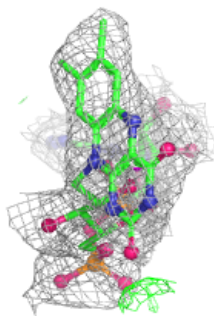
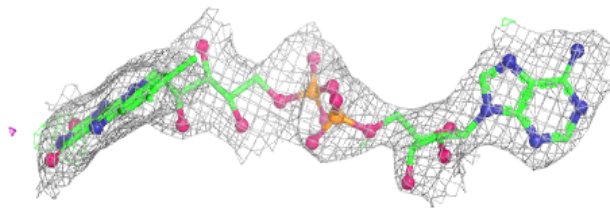
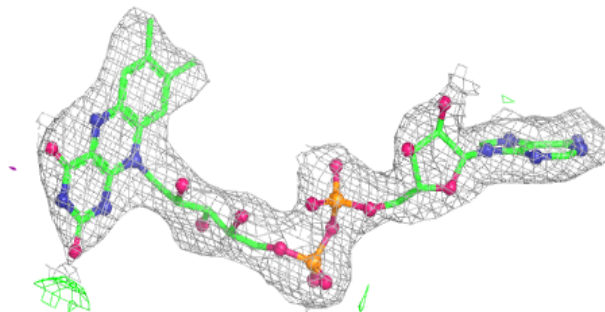


Electron density around FAD K 773:

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

**Electron density around FAD B 773:**

$2mF_o-DF_c$ (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.