



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 01:26 PM EDT

PDB ID : 3RED
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

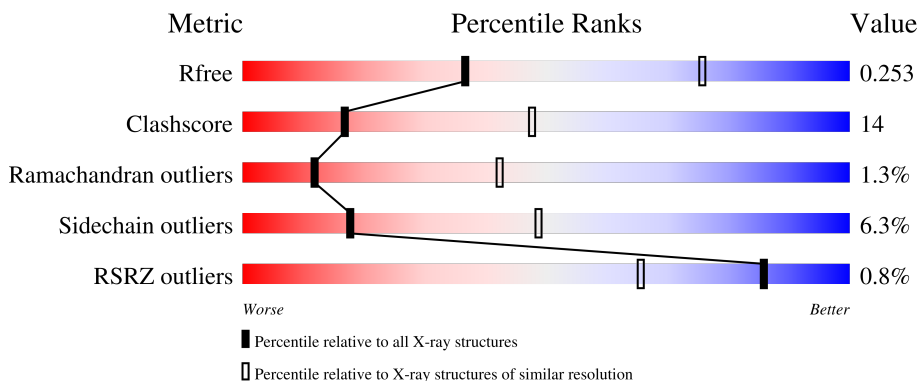
1 Overall quality at a glance

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}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (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	 72% 26%
1	B	521	 71% 26%
1	C	521	 76% 22%
1	D	521	 68% 28%
1	E	521	 76% 22%

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Mol	Chain	Length	Quality of chain
1	F	521	 % 69% 28% .
1	G	521	 % 70% 25% .
1	H	521	 % 70% 27% .
1	I	521	 % 70% 27% .
1	J	521	 % 71% 26% .
1	K	521	 % 70% 27% .
1	L	521	 % 64% 32% ..

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

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

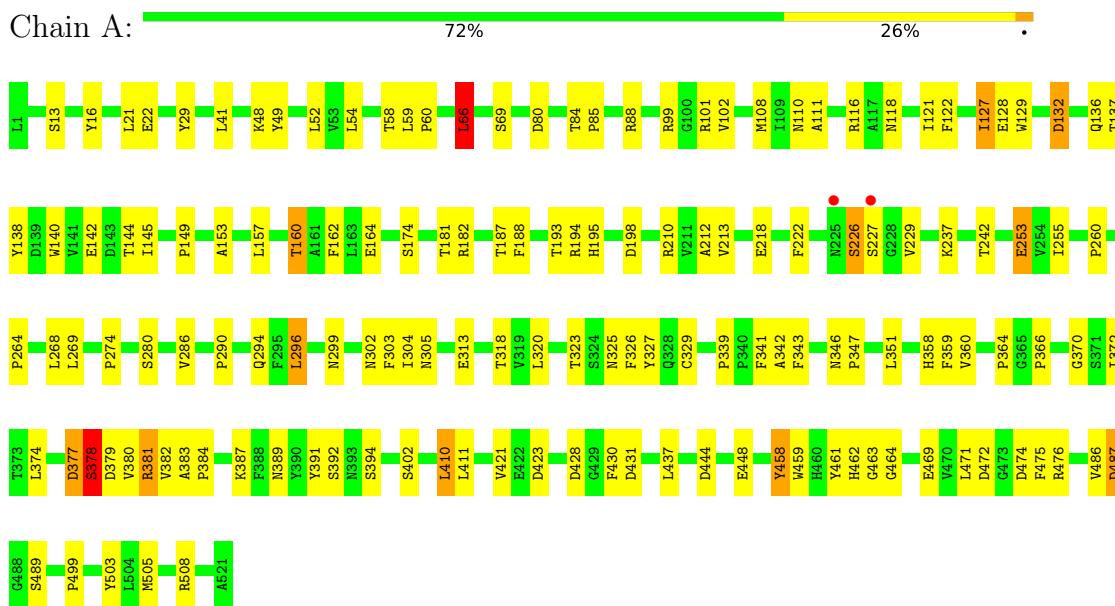


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0
2	C	1	53	27	9	15	2	0	0
2	D	1	53	27	9	15	2	0	0
2	E	1	53	27	9	15	2	0	0
2	F	1	53	27	9	15	2	0	0
2	G	1	53	27	9	15	2	0	0
2	H	1	53	27	9	15	2	0	0
2	I	1	53	27	9	15	2	0	0
2	J	1	53	27	9	15	2	0	0
2	K	1	53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

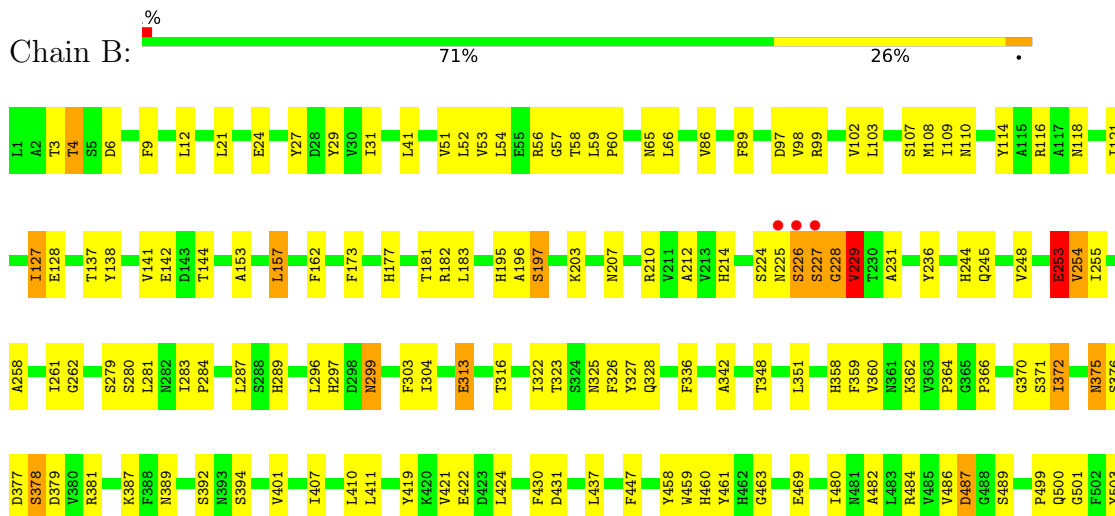
3 Residue-property plots

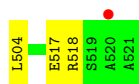
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

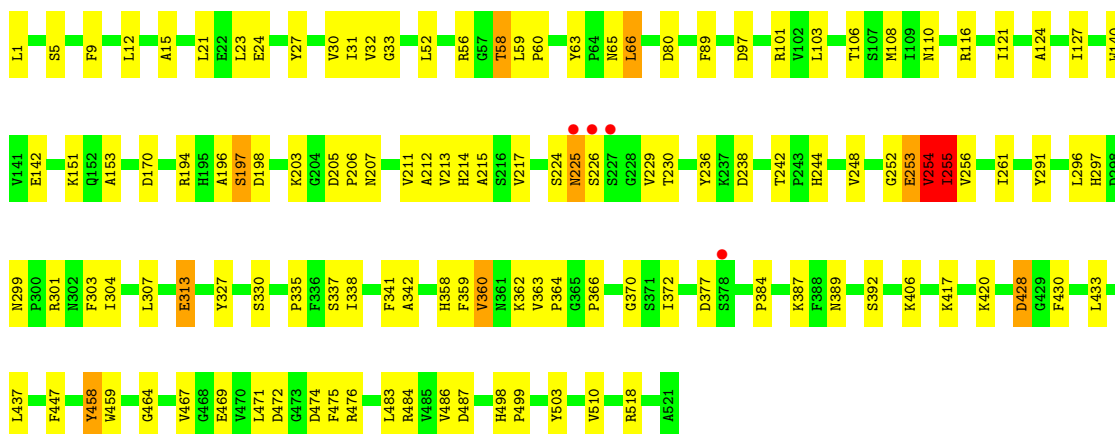
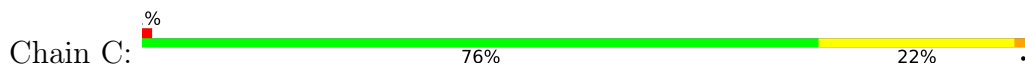


- Molecule 1: Hydroxynitrile lyase

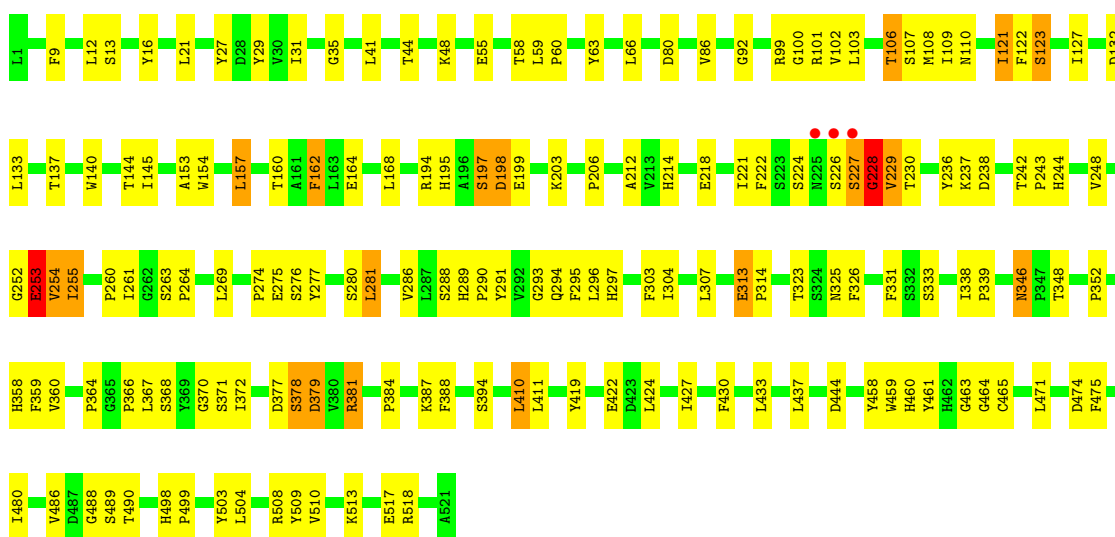




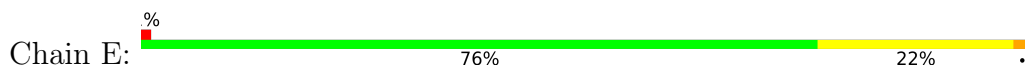
• Molecule 1: Hydroxynitrile lyase

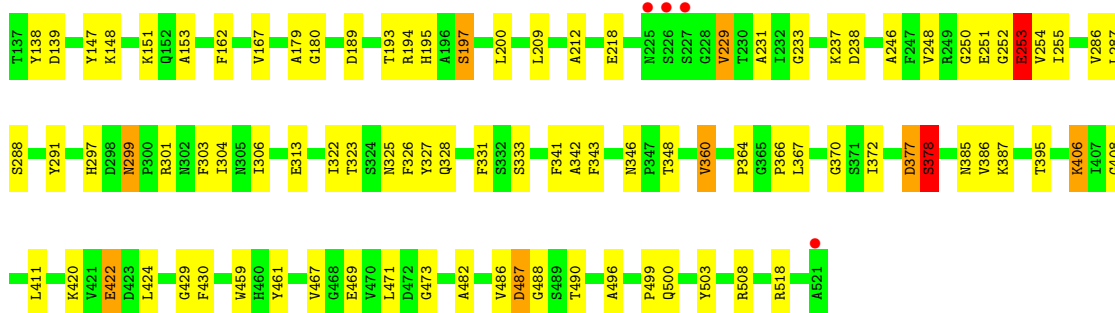


• Molecule 1: Hydroxynitrile lyase

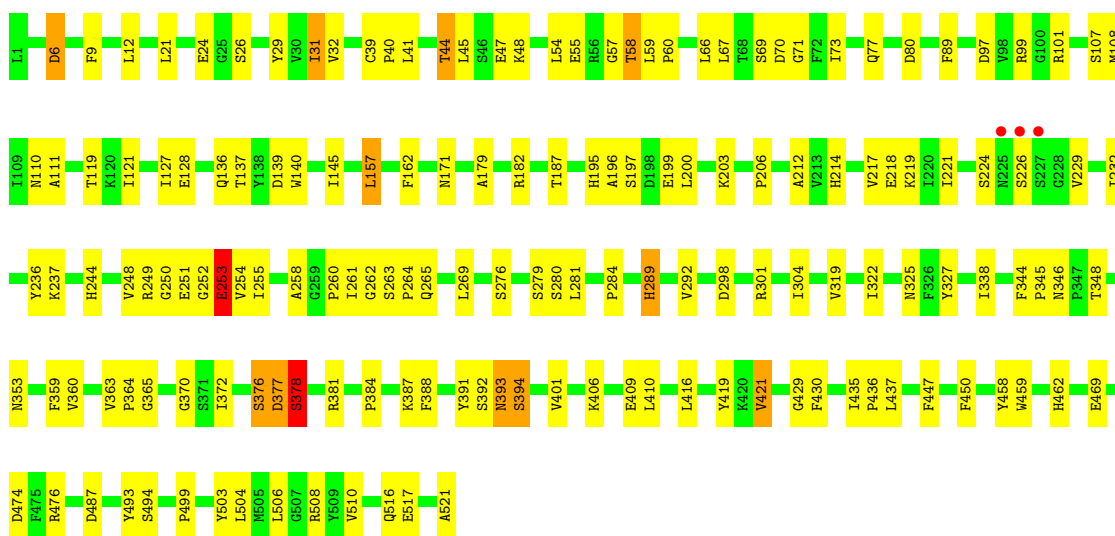


• Molecule 1: Hydroxynitrile lyase

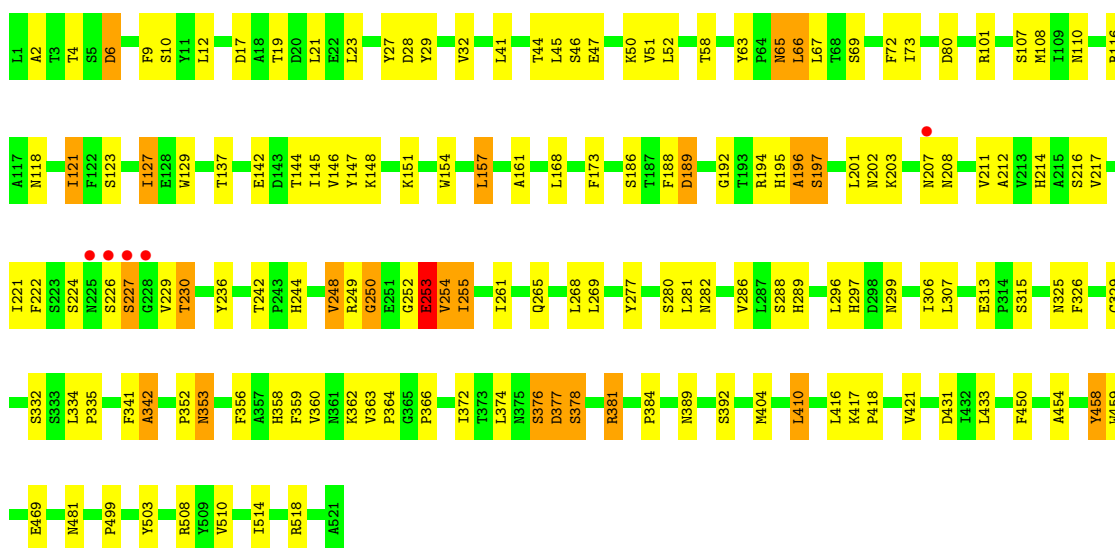




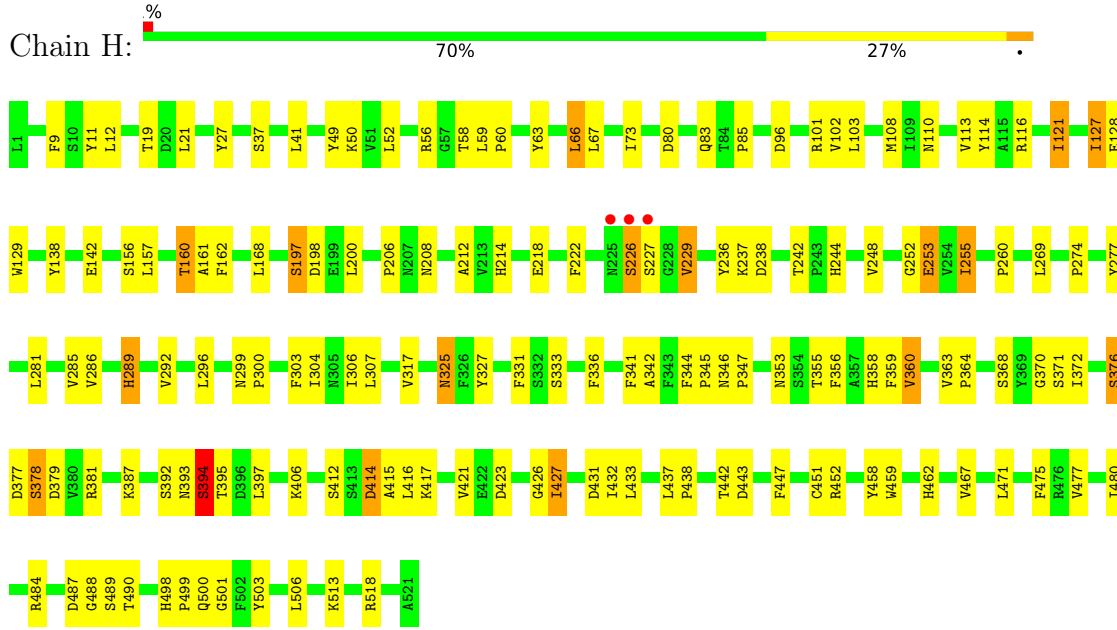
● Molecule 1: Hydroxynitrile lyase



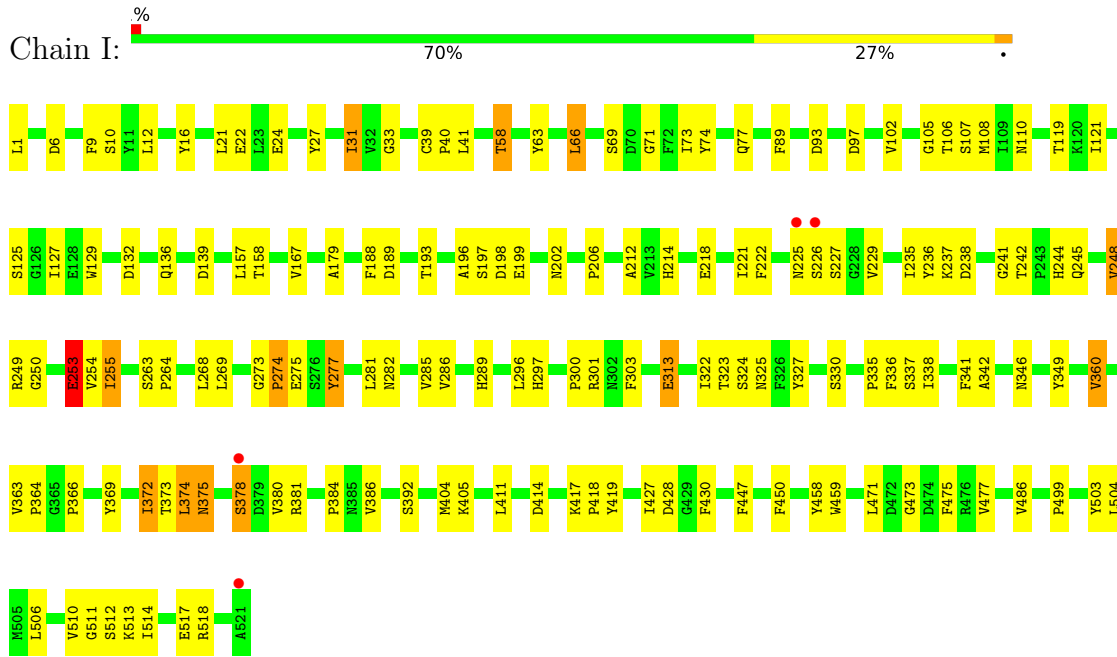
● Molecule 1: Hydroxynitrile lyase



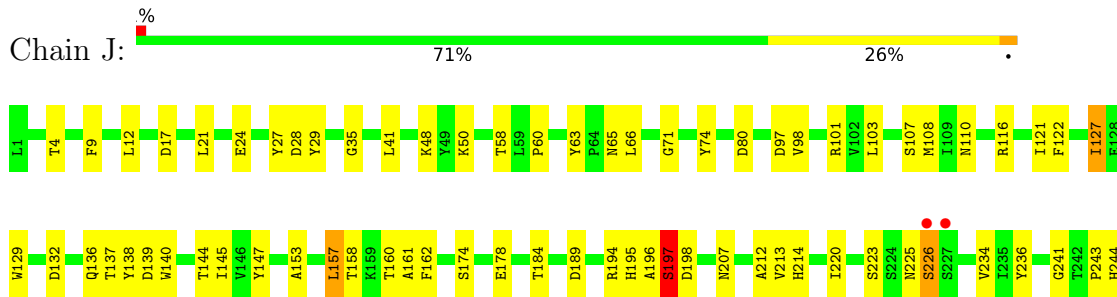
• Molecule 1: Hydroxynitrile lyase

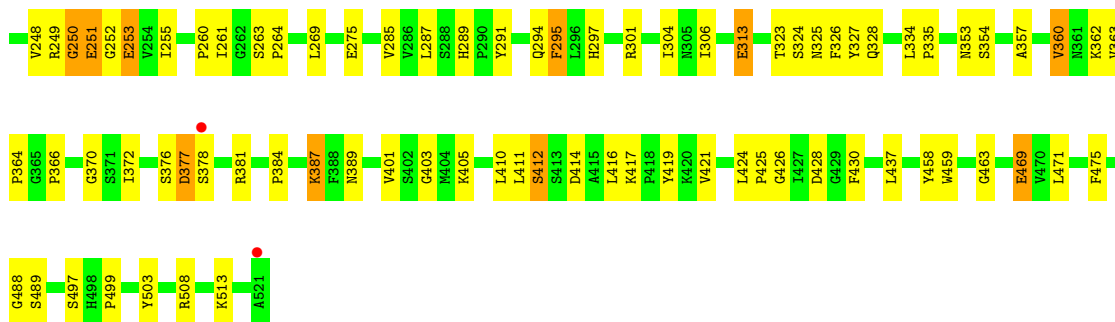


• Molecule 1: Hydroxynitrile lyase

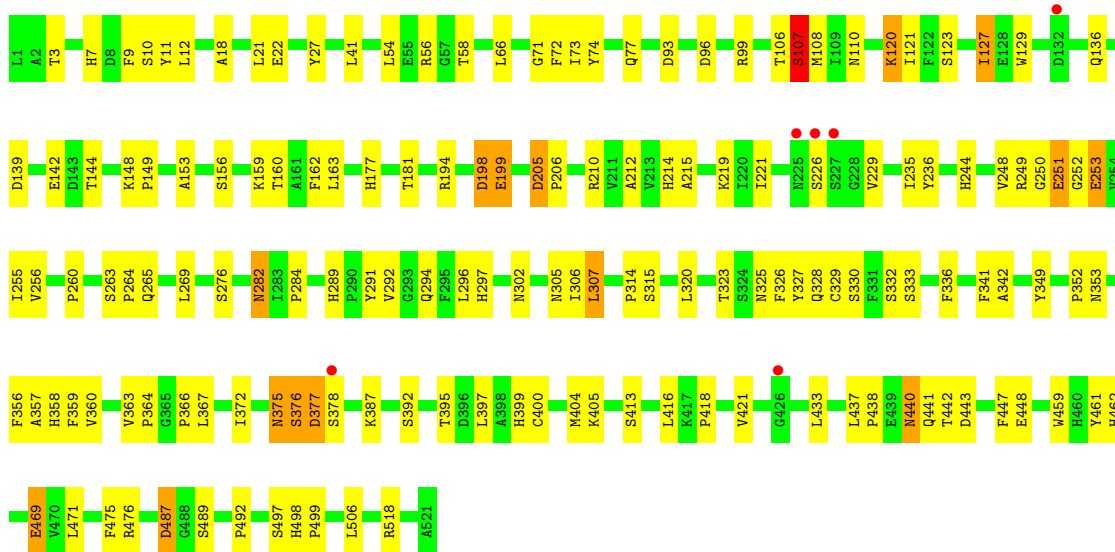


• Molecule 1: Hydroxynitrile lyase

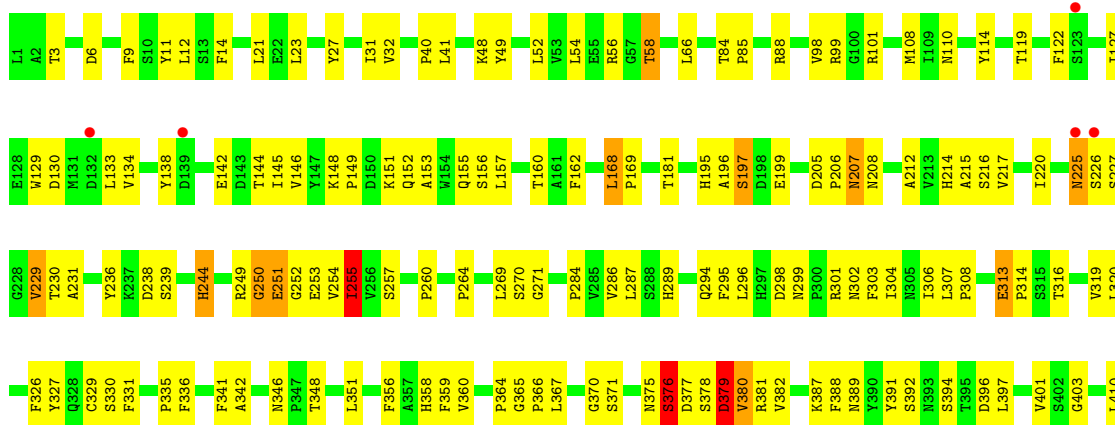


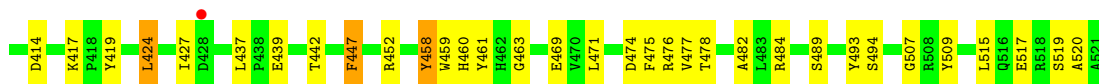


● Molecule 1: Hydroxynitrile lyase



● 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) 96.0 (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)	Xtrriage
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 (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	48604	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage'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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.69	0/4106	0.74	1/5606 (0.0%)
1	B	0.70	0/4107	0.77	1/5606 (0.0%)
1	C	0.69	1/4098 (0.0%)	0.74	1/5595 (0.0%)
1	D	0.78	2/4098 (0.0%)	0.80	5/5595 (0.1%)
1	E	0.71	0/4098	0.76	1/5595 (0.0%)
1	F	0.73	1/4109 (0.0%)	0.77	1/5609 (0.0%)
1	G	0.75	0/4109	0.77	1/5609 (0.0%)
1	H	0.75	3/4109 (0.1%)	0.76	1/5609 (0.0%)
1	I	0.72	0/4098	0.75	0/5595
1	J	0.70	0/4096	0.73	0/5593
1	K	0.76	3/4109 (0.1%)	0.75	1/5609 (0.0%)
1	L	0.77	2/4109 (0.0%)	0.73	3/5609 (0.1%)
All	All	0.73	12/49246 (0.0%)	0.76	16/67230 (0.0%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	195	HIS	CA-C	-5.44	1.38	1.52
1	L	254	VAL	CB-CG1	-5.41	1.41	1.52
1	C	24	GLU	CG-CD	5.38	1.60	1.51
1	D	198	ASP	CB-CG	-5.30	1.40	1.51
1	H	325	ASN	CG-OD1	5.18	1.35	1.24
1	K	387	LYS	CD-CE	5.14	1.64	1.51
1	F	391	TYR	CE2-CZ	-5.13	1.31	1.38
1	K	253	GLU	CG-CD	-5.09	1.44	1.51
1	K	375	ASN	CG-OD1	5.05	1.35	1.24
1	H	83	GLN	CD-OE1	5.03	1.35	1.24
1	L	207	ASN	CG-OD1	5.01	1.34	1.24
1	H	253	GLU	CD-OE1	-5.01	1.20	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	HIS	N-CA-C	-9.17	86.24	111.00
1	A	66	LEU	CB-CG-CD2	-6.69	99.62	111.00
1	D	157	LEU	CB-CG-CD1	-6.30	100.28	111.00
1	L	255	ILE	N-CA-C	-5.81	95.32	111.00
1	K	387	LYS	CD-CE-NZ	5.79	125.01	111.70
1	L	254	VAL	N-CA-C	-5.72	95.56	111.00
1	H	255	ILE	N-CA-C	-5.70	95.61	111.00
1	G	253	GLU	C-N-CA	5.65	135.82	121.70
1	B	253	GLU	C-N-CA	5.37	135.12	121.70
1	F	253	GLU	N-CA-C	-5.35	96.56	111.00
1	D	198	ASP	CB-CG-OD1	-5.17	113.65	118.30
1	C	254	VAL	N-CA-C	-5.16	97.08	111.00
1	D	253	GLU	C-N-CA	5.12	134.49	121.70
1	D	228	GLY	N-CA-C	-5.11	100.32	113.10
1	L	424	LEU	CA-CB-CG	5.05	126.92	115.30
1	E	253	GLU	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (14) planarity outliers are listed below:

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

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

5.2 Too-close contacts [i](#)

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	99	0
1	B	3999	0	3853	107	0
1	C	3993	0	3844	89	0
1	D	3993	0	3844	132	0
1	E	3993	0	3844	93	0
1	F	4001	0	3857	112	0
1	G	4001	0	3857	119	0
1	H	4001	0	3857	121	0
1	I	3993	0	3844	116	0
1	J	3991	0	3838	115	0
1	K	4001	0	3857	107	0
1	L	4001	0	3857	142	0
2	A	53	0	31	6	0
2	B	53	0	31	5	0
2	C	53	0	31	6	0
2	D	53	0	31	12	0
2	E	53	0	31	8	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	6	0
2	K	53	0	31	7	0
2	L	53	0	31	5	0
All	All	48604	0	46571	1342	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 14.

All (1342) 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: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: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:I:374:LEU:CA	1:I:375:ASN:HB2	1.98	0.93
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
1:A:21:LEU:HD11	1:A:212:ALA:HB2	1.53	0.91
1:H:377:ASP:N	1:H:378:SER:CA	2.33	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:376:SER:C	1:H:378:SER:HB2	1.95	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:F:252:GLY:C	1:F:253:GLU:HG2	1.95	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: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:C:252:GLY:C	1:C:253:GLU:CG	2.46	0.82
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
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:B:279:SER:C	1:B:281:LEU:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:252:GLY:C	1:C:253:GLU:HG2	2.03	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: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: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: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
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:F:80:ASP:CG	1:F:101:ARG:HH22	1.88	0.74
1:H:60:PRO:HB3	1:H:108:MET:HE2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:376:SER:C	1:H:378:SER:CB	2.57	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: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: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:H:376:SER:C	1:H:378:SER:HA	2.09	0.72
1:D:29:TYR:HA	1:D:253:GLU:O	1.88	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
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:D:227:SER:O	1:D:228:GLY:C	2.29	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:A:60:PRO:HB3	1:A:108:MET:HE2	1.71	0.71
1:C:110:ASN:HB2	2:C:773:FAD:C5X	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:252:GLY:C	1:G:253:GLU:HG2	2.12	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: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:E:107:SER:OG	1:E:197:SER:OG	2.11	0.69
1:B:227:SER:O	1:B:228:GLY:C	2.30	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: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
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:E:107:SER:HG	1:E:197:SER:HG	1.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:SER:C	1:H:378:SER:CA	2.62	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:G:195:HIS:C	1:G:196:ALA:O	2.30	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: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: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:J:60:PRO:HB3	1:J:108:MET:HE2	1.76	0.66
1:D:86:VAL:HG22	1:D:109:ILE:HD13	1.78	0.66
1:G:459:TRP:HB3	2:G:773:FAD:HM83	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:B:60:PRO:HB3	1:B:108:MET:HE2	1.77	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: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
1:A:269:LEU:HD22	1:A:378:SER:HA	1.78	0.65
1:B:279:SER:C	1:B:281:LEU:N	2.51	0.64
1:D:293:GLY:CA	1:D:372:ILE:HG22	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:GLN:O	1:D:464:GLY:HA2	1.97	0.64
1:H:11:TYR:OH	1:H:198:ASP:OD2	2.06	0.64
1:I:301:ARG:HB2	1:I:458:TYR:CD1	2.32	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:106:THR:C	1:K:108:MET:H	2.04	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: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:J:377:ASP:H	1:J:378:SER:C	2.05	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:K:106:THR:O	1:K:107:SER:C	2.38	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:K:106:THR:C	1:K:108:MET:N	2.55	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: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
1:C:304:ILE:HD11	1:C:437:LEU:HG	1.83	0.59
1:J:27:TYR:O	1:J:248:VAL:HA	2.02	0.59
1:J:80:ASP:OD1	1:J:101:ARG:NH2	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:60:PRO:HB3	1:H:108:MET:CE	2.33	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:B:60:PRO:HB3	1:B:108:MET:CE	2.32	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:A:459:TRP:HB3	2:A:773:FAD:HM83	1.85	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
1:C:301:ARG:HD2	1:C:360:VAL:HG11	1.85	0.57
1:L:294:GLN:O	1:L:295:PHE:HB2	2.04	0.57
1:G:9:PHE:HB3	1:G:12:LEU:HD12	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:252:GLY:C	1:J:253:GLU:HG2	2.25	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
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:C:252:GLY:C	1:C:253:GLU:HG3	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:252:GLY:C	1:H:253:GLU:CG	2.75	0.54
1:A:160:THR:O	1:A:164:GLU:HG3	2.06	0.54
1:D:458:TYR:O	1:D:459:TRP:HB2	2.08	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: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:D:252:GLY:C	1:D:253:GLU:HG2	2.28	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:A:459:TRP:HB3	2:A:773:FAD:C8M	2.37	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: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: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: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
1:D:486:VAL:CG2	1:D:510:VAL:HG11	2.35	0.53
1:E:60:PRO:HB3	1:E:108:MET:HE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:PRO:HD3	1:D:103:LEU:HB3	1.90	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: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: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: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:60:PRO:HB3	1:J:108:MET:CE	2.40	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:H:500:GLN:O	1:H:501:GLY:C	2.48	0.52
1:K:252:GLY:C	1:K:253:GLU:CG	2.77	0.52
1:L:157:LEU:CD1	1:L:419:TYR:OH	2.58	0.52
1:J:301:ARG:HG3	1:J:360:VAL:HG12	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:377:ASP:N	1:L:378:SER:CA	2.55	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:G:226:SER:HA	1:G:227:SER:C	2.31	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
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: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:K:359:PHE:CZ	1:K:416:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:60:PRO:HB3	1:C:108:MET:HE2	1.92	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:459:TRP:HB3	2:B:773:FAD:HM83	1.94	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: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: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:313:GLU:CD	1:D:313:GLU:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:375:ASN:OD1	1:L:375:ASN:N	2.43	0.49
1:L:377:ASP:N	1:L:378:SER:C	2.66	0.49
1:B:228:GLY:O	1:B:229:VAL:C	2.49	0.49
1:H:226:SER:HA	1:H:227:SER:C	2.31	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:J:122:PHE:HZ	1:J:138:TYR:HH	1.59	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:F:376:SER:O	1:F:377:ASP:C	2.50	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
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:73:ILE:HD12	1:I:336:PHE:CE2	2.48	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: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:E:252:GLY:C	1:E:253:GLU:HG2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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
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:D:227:SER:C	1:D:228:GLY:O	2.51	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:376:SER:CB	1:H:378:SER:HB2	2.44	0.48
1:B:225:ASN:HA	1:B:227:SER:HA	1.96	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:L:377:ASP:H	1:L:378:SER:C	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:3:THR:O	1:B:4:THR:C	2.53	0.47
1:D:121:ILE:C	1:D:123:SER:H	2.18	0.47
1:E:136:GLN:O	1:E:139:ASP:HB2	2.15	0.47
1:I:189:ASP:C	1:I:189:ASP:OD2	2.53	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
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:60:PRO:HB3	1:C:108:MET:CE	2.45	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:K:333:SER:HG	1:K:336:PHE:HE2	1.62	0.47
1:L:302:ASN:ND2	1:L:391:TYR:OH	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:195:HIS:C	1:B:196:ALA:O	2.52	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
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:377:ASP:N	1:J:378:SER:C	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:376:SER:HG	1:H:379:ASP:H	1.63	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:B:486:VAL:O	1:B:487:ASP:HB3	2.16	0.46
1:G:45:LEU:C	1:G:47:GLU:H	2.18	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:C:9:PHE:HB3	1:C:12:LEU:HD12	1.97	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:222:PHE:CD1	1:I:286:VAL:HG11	2.50	0.46
1:K:320:LEU:HD23	1:K:329:CYS:HB3	1.96	0.46
1:F:450:PHE:C	1:F:450:PHE:CD2	2.88	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:K:71:GLY:O	1:K:72:PHE:C	2.53	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: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:69:SER:C	1:F:71:GLY:H	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:458:TYR:O	1:A:459:TRP:HB2	2.16	0.45
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: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
1:I:125:SER:HG	1:I:129:TRP:HE1	1.65	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:K:205:ASP:C	1:K:205:ASP:OD1	2.53	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: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: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:E:459:TRP:HB3	2:E:773:FAD:HM83	1.98	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:66:LEU:HD12	1:L:66:LEU:C	2.36	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:D:255:ILE:HD11	1:D:486:VAL:HB	1.98	0.45
1:E:287:LEU:HG	1:E:288:SER:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:337:SER:C	1:I:338:ILE:HG13	2.37	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: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
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: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:L:114:TYR:C	1:L:114:TYR:CD2	2.90	0.45
1:D:293:GLY:HA2	1:D:372:ILE:CG2	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:I:106:THR:HG22	1:I:106:THR:O	2.17	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: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:E:377:ASP:HB2	1:E:378:SER:CB	2.47	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: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:22:GLU:CD	1:I:22:GLU:H	2.20	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:B:389:ASN:HB3	1:B:392:SER:HG	1.82	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: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:I:313:GLU:CD	1:I:313:GLU:H	2.21	0.44
1:A:142:GLU:C	1:A:144:THR:H	2.21	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: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:E:238:ASP:OD1	1:E:238:ASP:C	2.57	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:H:378:SER:OG	1:H:379:ASP:C	2.57	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: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:E:37:SER:C	1:E:40:PRO:HD2	2.37	0.43
1:G:249:ARG:O	1:G:250:GLY:C	2.57	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: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:252:GLY:C	1:H:253:GLU:HG3	2.38	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:B:66:LEU:CD1	1:B:108:MET:HE2	2.49	0.43
1:D:162:PHE:HD2	1:D:410:LEU:HD11	1.83	0.43
1:F:69:SER:C	1:F:71:GLY:N	2.72	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: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: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: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: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: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:C:153:ALA:HB3	1:C:313:GLU:CD	2.40	0.43
1:C:487:ASP:OD2	1:C:487:ASP:C	2.57	0.43
1:D:198:ASP:OD1	1:D:198:ASP:C	2.40	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: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
1:B:58:THR:HG23	1:B:214:HIS:HE1	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:K:459:TRP:HB3	2:K:773:FAD:HM83	2.02	0.42
1:L:152:GLN:O	1:L:153:ALA:C	2.57	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:F:249:ARG:O	1:F:250:GLY:C	2.58	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:HG3	1:D:108:MET:O	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
1:J:362:LYS:HB2	1:J:458:TYR:CE1	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:223:SER:C	1:J:225:ASN:H	2.23	0.42
1:L:302:ASN:HD21	1:L:391:TYR:HH	1.63	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:G:189:ASP:C	1:G:189:ASP:OD2	2.57	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:E:299:ASN:CG	1:E:366:PRO:HD3	2.40	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:205:ASP:OD1	1:L:207:ASN:N	2.52	0.41
1:B:56:ARG:HG3	1:B:57:GLY:N	2.35	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:B:460:HIS:O	1:B:461:TYR:C	2.57	0.41

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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	0.41
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:D:379:ASP:C	1:D:381:ARG:N	2.74	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:I:69:SER:C	1:I:71:GLY:H	2.23	0.41
1:I:369:TYR:CD1	1:I:369:TYR:C	2.93	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:J:249:ARG:O	1:J:250:GLY:C	2.59	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:H:289:HIS:HB3	1:H:292:VAL:HG23	2.01	0.41
1:I:249:ARG:O	1:I:250:GLY:C	2.58	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:252:GLY:C	1:K:253:GLU:HG3	2.41	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:L:379:ASP:C	1:L:381:ARG:N	2.72	0.41
1:L:474:ASP:O	1:L:475:PHE:HB2	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:C:66:LEU:HD13	1:C:108:MET:HE2	2.03	0.41
1:D:110:ASN:HA	2:D:773:FAD:C6	2.51	0.41
1:E:106:THR:HG1	2:E:773:FAD:PA	2.43	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:K:142:GLU:C	1:K:144:THR:H	2.24	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:189:ASP:OD2	1:E:189:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:472:ASP:OD1	1:A:472:ASP:C	2.60	0.41
1:B:89:PHE:CE2	1:B:97:ASP:HB3	2.56	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:60:PRO:HB3	1:F:108:MET:HE2	2.03	0.41
1:F:218:GLU:OE2	1:F:237:LYS:CD	2.67	0.41
1:F:279:SER:C	1:F:281:LEU:H	2.24	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:L:459:TRP:HB3	2:L:773:FAD:HM83	2.03	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	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:127:ILE:O	1:B:127:ILE:HG13	2.22	0.40
1:C:103:LEU:CD2	1:C:211:VAL:HG11	2.51	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: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%)	15	49
1	B	521/521 (100%)	474 (91%)	36 (7%)	11 (2%)	7	30
1	C	520/521 (100%)	476 (92%)	39 (8%)	5 (1%)	15	49
1	D	520/521 (100%)	470 (90%)	42 (8%)	8 (2%)	10	39
1	E	520/521 (100%)	482 (93%)	34 (6%)	4 (1%)	19	54
1	F	521/521 (100%)	476 (91%)	37 (7%)	8 (2%)	10	39
1	G	521/521 (100%)	479 (92%)	32 (6%)	10 (2%)	8	33
1	H	521/521 (100%)	485 (93%)	30 (6%)	6 (1%)	13	44
1	I	520/521 (100%)	481 (92%)	33 (6%)	6 (1%)	13	44
1	J	520/521 (100%)	480 (92%)	35 (7%)	5 (1%)	15	49
1	K	521/521 (100%)	466 (89%)	45 (9%)	10 (2%)	8	33
1	L	521/521 (100%)	476 (91%)	38 (7%)	7 (1%)	12	42
All	All	6247/6252 (100%)	5730 (92%)	432 (7%)	85 (1%)	12	40

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	442/440 (100%)	416 (94%)	26 (6%)	19	51
1	B	441/440 (100%)	416 (94%)	25 (6%)	20	53
1	C	441/440 (100%)	417 (95%)	24 (5%)	22	55
1	D	441/440 (100%)	409 (93%)	32 (7%)	14	42
1	E	441/440 (100%)	422 (96%)	19 (4%)	29	63
1	F	442/440 (100%)	413 (93%)	29 (7%)	16	47
1	G	442/440 (100%)	409 (92%)	33 (8%)	13	41
1	H	442/440 (100%)	410 (93%)	32 (7%)	14	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	441/440 (100%)	415 (94%)	26 (6%)	19	51
1	J	439/440 (100%)	415 (94%)	24 (6%)	21	54
1	K	442/440 (100%)	413 (93%)	29 (7%)	16	47
1	L	442/440 (100%)	405 (92%)	37 (8%)	11	36
All	All	5296/5280 (100%)	4960 (94%)	336 (6%)	18	49

All (336) 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	127	ILE
1	A	132	ASP
1	A	157	LEU
1	A	160	THR
1	A	193	THR
1	A	226	SER
1	A	229	VAL
1	A	242	THR
1	A	253	GLU
1	A	280	SER
1	A	296	LEU
1	A	323	THR
1	A	372	ILE
1	A	377	ASP
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	458	TYR
1	A	469	GLU
1	B	65	ASN
1	B	127	ILE
1	B	157	LEU
1	B	207	ASN
1	B	224	SER
1	B	226	SER

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Mol	Chain	Res	Type
1	B	227	SER
1	B	229	VAL
1	B	254	VAL
1	B	289	HIS
1	B	296	LEU
1	B	299	ASN
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	458	TYR
1	B	469	GLU
1	B	517	GLU
1	B	518	ARG
1	C	1	LEU
1	C	23	LEU
1	C	58	THR
1	C	65	ASN
1	C	66	LEU
1	C	121	ILE
1	C	127	ILE
1	C	151	LYS
1	C	207	ASN
1	C	224	SER
1	C	225	ASN
1	C	229	VAL
1	C	230	THR
1	C	254	VAL
1	C	255	ILE
1	C	313	GLU
1	C	360	VAL
1	C	372	ILE
1	C	377	ASP
1	C	406	LYS
1	C	417	LYS
1	C	428	ASP
1	C	458	TYR

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Mol	Chain	Res	Type
1	C	518	ARG
1	D	13	SER
1	D	31	ILE
1	D	106	THR
1	D	121	ILE
1	D	123	SER
1	D	127	ILE
1	D	132	ASP
1	D	162	PHE
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	276	SER
1	D	281	LEU
1	D	313	GLU
1	D	314	PRO
1	D	323	THR
1	D	346	ASN
1	D	368	SER
1	D	371	SER
1	D	379	ASP
1	D	381	ARG
1	D	394	SER
1	D	410	LEU
1	D	427	ILE
1	D	444	ASP
1	D	518	ARG
1	E	3	THR
1	E	121	ILE
1	E	151	LYS
1	E	162	PHE
1	E	193	THR
1	E	197	SER
1	E	229	VAL
1	E	299	ASN
1	E	306	ILE

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Mol	Chain	Res	Type
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	406	LYS
1	E	422	GLU
1	E	518	ARG
1	F	6	ASP
1	F	26	SER
1	F	31	ILE
1	F	44	THR
1	F	58	THR
1	F	66	LEU
1	F	70	ASP
1	F	121	ILE
1	F	127	ILE
1	F	157	LEU
1	F	171	ASN
1	F	224	SER
1	F	226	SER
1	F	229	VAL
1	F	251	GLU
1	F	253	GLU
1	F	276	SER
1	F	289	HIS
1	F	338	ILE
1	F	372	ILE
1	F	376	SER
1	F	378	SER
1	F	392	SER
1	F	393	ASN
1	F	421	VAL
1	F	469	GLU
1	F	494	SER
1	F	516	GLN
1	F	517	GLU
1	G	6	ASP
1	G	23	LEU
1	G	65	ASN

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Mol	Chain	Res	Type
1	G	66	LEU
1	G	121	ILE
1	G	127	ILE
1	G	151	LYS
1	G	157	LEU
1	G	168	LEU
1	G	189	ASP
1	G	207	ASN
1	G	221	ILE
1	G	224	SER
1	G	227	SER
1	G	229	VAL
1	G	230	THR
1	G	242	THR
1	G	248	VAL
1	G	254	VAL
1	G	255	ILE
1	G	280	SER
1	G	288	SER
1	G	289	HIS
1	G	313	GLU
1	G	353	ASN
1	G	376	SER
1	G	381[A]	ARG
1	G	381[B]	ARG
1	G	410	LEU
1	G	458	TYR
1	G	469	GLU
1	G	481	ASN
1	G	518	ARG
1	H	37	SER
1	H	66	LEU
1	H	121	ILE
1	H	127	ILE
1	H	128	GLU
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

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Mol	Chain	Res	Type
1	H	242	THR
1	H	281	LEU
1	H	285	VAL
1	H	289	HIS
1	H	296	LEU
1	H	355	THR
1	H	360	VAL
1	H	371	SER
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	414	ASP
1	H	416	LEU
1	H	427	ILE
1	H	442	THR
1	H	458	TYR
1	H	518	ARG
1	I	6	ASP
1	I	31	ILE
1	I	58	THR
1	I	66	LEU
1	I	93	ASP
1	I	119	THR
1	I	121	ILE
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	360	VAL
1	I	372	ILE
1	I	373	THR
1	I	374	LEU
1	I	380	VAL
1	I	381	ARG
1	I	392	SER

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Mol	Chain	Res	Type
1	I	427	ILE
1	I	428	ASP
1	I	512	SER
1	I	518	ARG
1	J	24	GLU
1	J	121	ILE
1	J	127	ILE
1	J	132	ASP
1	J	157	LEU
1	J	160	THR
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	412	SER
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	198	ASP
1	K	199	GLU
1	K	205	ASP
1	K	219	LYS
1	K	226	SER
1	K	229	VAL

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Mol	Chain	Res	Type
1	K	249	ARG
1	K	251	GLU
1	K	276	SER
1	K	282	ASN
1	K	296	LEU
1	K	307	LEU
1	K	315	SER
1	K	323	THR
1	K	372	ILE
1	K	377	ASP
1	K	392	SER
1	K	421	VAL
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	58	THR
1	L	119	THR
1	L	156	SER
1	L	160	THR
1	L	168	LEU
1	L	225	ASN
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
1	L	360	VAL
1	L	367	LEU
1	L	371	SER
1	L	376	SER
1	L	379	ASP
1	L	380	VAL
1	L	394	SER
1	L	414	ASP

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Mol	Chain	Res	Type
1	L	417	LYS
1	L	424	LEU
1	L	427	ILE
1	L	439	GLU
1	L	442	THR
1	L	447	PHE
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	195	HIS
1	I	385	ASN
1	J	195	HIS
1	K	214	HIS
1	K	305	ASN
1	K	441	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	D	773	-	53,58,58	1.15	4 (7%)	68,89,89	1.45	9 (13%)
2	FAD	H	773	-	53,58,58	1.23	3 (5%)	68,89,89	1.55	12 (17%)
2	FAD	I	773	-	53,58,58	1.19	4 (7%)	68,89,89	1.46	12 (17%)
2	FAD	G	773	-	53,58,58	1.22	5 (9%)	68,89,89	1.55	14 (20%)
2	FAD	J	773	-	53,58,58	1.15	4 (7%)	68,89,89	1.50	10 (14%)
2	FAD	F	773	-	53,58,58	1.18	4 (7%)	68,89,89	1.46	9 (13%)
2	FAD	K	773	-	53,58,58	1.12	4 (7%)	68,89,89	1.39	8 (11%)
2	FAD	L	773	-	53,58,58	1.22	4 (7%)	68,89,89	1.48	12 (17%)
2	FAD	C	773	-	53,58,58	1.20	4 (7%)	68,89,89	1.48	11 (16%)
2	FAD	E	773	-	53,58,58	1.32	4 (7%)	68,89,89	1.39	12 (17%)
2	FAD	A	773	-	53,58,58	1.22	5 (9%)	68,89,89	1.41	13 (19%)
2	FAD	B	773	-	53,58,58	1.15	4 (7%)	68,89,89	1.36	12 (17%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	773	-	-	3/30/50/50	0/6/6/6
2	FAD	H	773	-	-	4/30/50/50	0/6/6/6
2	FAD	I	773	-	-	3/30/50/50	0/6/6/6
2	FAD	G	773	-	-	9/30/50/50	0/6/6/6
2	FAD	J	773	-	-	2/30/50/50	0/6/6/6
2	FAD	F	773	-	-	6/30/50/50	0/6/6/6
2	FAD	K	773	-	-	8/30/50/50	0/6/6/6
2	FAD	L	773	-	-	3/30/50/50	0/6/6/6
2	FAD	C	773	-	-	8/30/50/50	0/6/6/6
2	FAD	E	773	-	-	7/30/50/50	0/6/6/6
2	FAD	A	773	-	-	12/30/50/50	0/6/6/6
2	FAD	B	773	-	-	10/30/50/50	0/6/6/6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	773	FAD	C4X-N5	5.17	1.40	1.30
2	I	773	FAD	C2A-N3A	4.72	1.39	1.32
2	A	773	FAD	C4X-N5	4.58	1.39	1.30
2	E	773	FAD	C2A-N3A	4.56	1.39	1.32
2	H	773	FAD	C2A-N3A	4.48	1.39	1.32
2	C	773	FAD	C4X-N5	4.23	1.39	1.30
2	F	773	FAD	C4X-N5	4.09	1.38	1.30
2	D	773	FAD	C2A-N3A	4.06	1.38	1.32
2	L	773	FAD	C2A-N3A	4.00	1.38	1.32
2	I	773	FAD	C4X-N5	3.97	1.38	1.30
2	K	773	FAD	C2A-N3A	3.91	1.38	1.32
2	L	773	FAD	C4X-N5	3.90	1.38	1.30
2	F	773	FAD	C2A-N3A	3.80	1.38	1.32
2	K	773	FAD	C4X-N5	3.73	1.38	1.30
2	J	773	FAD	C4X-N5	3.72	1.38	1.30
2	G	773	FAD	C4X-N5	3.68	1.37	1.30
2	L	773	FAD	C10-N1	3.63	1.40	1.33
2	D	773	FAD	C4X-N5	3.60	1.37	1.30
2	B	773	FAD	C2A-N3A	3.58	1.37	1.32
2	J	773	FAD	C2A-N3A	3.48	1.37	1.32
2	G	773	FAD	C2A-N3A	3.40	1.37	1.32
2	J	773	FAD	C10-N1	3.38	1.40	1.33
2	A	773	FAD	C2A-N3A	3.27	1.37	1.32
2	C	773	FAD	C2A-N3A	3.27	1.37	1.32
2	A	773	FAD	C2A-N1A	3.22	1.39	1.33
2	H	773	FAD	C4X-N5	3.20	1.37	1.30
2	B	773	FAD	C4X-N5	3.18	1.36	1.30
2	G	773	FAD	C10-N1	3.16	1.39	1.33
2	H	773	FAD	C2A-N1A	2.99	1.39	1.33
2	F	773	FAD	C10-N1	2.89	1.39	1.33
2	C	773	FAD	C10-N1	2.78	1.38	1.33
2	F	773	FAD	C2A-N1A	2.72	1.39	1.33
2	D	773	FAD	C10-N1	2.72	1.38	1.33
2	E	773	FAD	C2A-N1A	2.70	1.38	1.33
2	E	773	FAD	C10-N1	2.70	1.38	1.33
2	B	773	FAD	C2A-N1A	2.67	1.38	1.33
2	A	773	FAD	C10-N1	2.61	1.38	1.33
2	D	773	FAD	C2A-N1A	2.60	1.38	1.33
2	K	773	FAD	C2A-N1A	2.58	1.38	1.33
2	I	773	FAD	C2A-N1A	2.55	1.38	1.33
2	G	773	FAD	C2A-N1A	2.54	1.38	1.33
2	G	773	FAD	C5'-C4'	2.47	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	773	FAD	C10-N1	2.39	1.38	1.33
2	L	773	FAD	C2A-N1A	2.38	1.38	1.33
2	J	773	FAD	C2A-N1A	2.27	1.38	1.33
2	C	773	FAD	C2A-N1A	2.19	1.38	1.33
2	K	773	FAD	C10-N1	2.19	1.37	1.33
2	A	773	FAD	O4B-C4B	-2.09	1.40	1.45
2	I	773	FAD	C10-N1	2.03	1.37	1.33

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	773	FAD	N3A-C2A-N1A	-6.10	119.15	128.68
2	F	773	FAD	N3A-C2A-N1A	-5.90	119.46	128.68
2	J	773	FAD	N3A-C2A-N1A	-5.63	119.87	128.68
2	D	773	FAD	N3A-C2A-N1A	-5.56	119.98	128.68
2	G	773	FAD	N3A-C2A-N1A	-5.42	120.21	128.68
2	L	773	FAD	N3A-C2A-N1A	-5.39	120.25	128.68
2	I	773	FAD	N3A-C2A-N1A	-4.94	120.95	128.68
2	A	773	FAD	N3A-C2A-N1A	-4.79	121.19	128.68
2	B	773	FAD	N3A-C2A-N1A	-4.48	121.67	128.68
2	H	773	FAD	N3A-C2A-N1A	-4.33	121.90	128.68
2	K	773	FAD	N3A-C2A-N1A	-4.31	121.94	128.68
2	E	773	FAD	N3A-C2A-N1A	-4.25	122.04	128.68
2	H	773	FAD	C4X-C10-N10	4.05	122.40	116.48
2	F	773	FAD	C4-N3-C2	-3.58	119.03	125.64
2	I	773	FAD	C4-N3-C2	-3.58	119.03	125.64
2	D	773	FAD	O4-C4-C4X	-3.45	117.44	126.60
2	D	773	FAD	C4-N3-C2	-3.41	119.35	125.64
2	H	773	FAD	C10-C4X-N5	-3.37	117.71	124.86
2	G	773	FAD	C4X-C10-N10	3.31	121.32	116.48
2	L	773	FAD	C4X-C10-N1	-3.27	117.14	124.73
2	H	773	FAD	O2-C2-N1	-3.20	116.53	121.83
2	L	773	FAD	C4X-C4-N3	3.19	121.29	113.19
2	L	773	FAD	C10-C4X-N5	-3.17	118.12	124.86
2	K	773	FAD	P-O3P-PA	-3.16	121.97	132.83
2	C	773	FAD	P-O3P-PA	-3.14	122.06	132.83
2	L	773	FAD	C4-N3-C2	-3.12	119.88	125.64
2	K	773	FAD	C4A-C5A-N7A	-3.10	106.17	109.40
2	H	773	FAD	P-O3P-PA	-3.10	122.20	132.83
2	I	773	FAD	P-O3P-PA	-3.04	122.38	132.83
2	E	773	FAD	P-O3P-PA	-3.04	122.39	132.83
2	G	773	FAD	P-O3P-PA	-3.03	122.42	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	773	FAD	C4-N3-C2	-3.03	120.04	125.64
2	G	773	FAD	C4-C4X-N5	3.03	122.54	118.23
2	G	773	FAD	C4X-C4-N3	3.02	120.86	113.19
2	F	773	FAD	C4X-C4-N3	2.96	120.71	113.19
2	J	773	FAD	C4-N3-C2	-2.95	120.18	125.64
2	G	773	FAD	C10-N1-C2	2.94	122.79	116.90
2	H	773	FAD	C4-C4X-N5	2.90	122.37	118.23
2	A	773	FAD	C4-N3-C2	-2.90	120.29	125.64
2	E	773	FAD	O3B-C3B-C4B	-2.89	102.69	111.05
2	D	773	FAD	P-O3P-PA	-2.89	122.91	132.83
2	G	773	FAD	C4-N3-C2	-2.87	120.33	125.64
2	D	773	FAD	C4X-C4-N3	2.84	120.40	113.19
2	I	773	FAD	O2-C2-N1	-2.82	117.16	121.83
2	I	773	FAD	O4-C4-C4X	-2.81	119.14	126.60
2	C	773	FAD	C4X-C4-N3	2.81	120.31	113.19
2	L	773	FAD	C10-N1-C2	2.80	122.50	116.90
2	C	773	FAD	O4-C4-C4X	-2.79	119.21	126.60
2	H	773	FAD	C4-N3-C2	-2.77	120.52	125.64
2	G	773	FAD	C4A-C5A-N7A	-2.77	106.51	109.40
2	B	773	FAD	C4X-C4-N3	2.76	120.19	113.19
2	J	773	FAD	O3B-C3B-C4B	-2.75	103.10	111.05
2	H	773	FAD	O4B-C1B-C2B	-2.75	102.91	106.93
2	L	773	FAD	C4X-C10-N10	2.74	120.48	116.48
2	F	773	FAD	C4X-C10-N1	-2.73	118.39	124.73
2	G	773	FAD	C10-C4X-N5	-2.73	119.07	124.86
2	B	773	FAD	P-O3P-PA	-2.73	123.47	132.83
2	B	773	FAD	C4X-C10-N1	-2.72	118.41	124.73
2	L	773	FAD	P-O3P-PA	-2.72	123.50	132.83
2	J	773	FAD	O5'-C5'-C4'	-2.69	102.17	109.36
2	I	773	FAD	C4X-C10-N10	2.67	120.39	116.48
2	A	773	FAD	C5X-C9A-N10	2.67	120.71	117.95
2	I	773	FAD	C9A-C5X-N5	-2.67	119.53	122.43
2	G	773	FAD	O4-C4-C4X	-2.66	119.53	126.60
2	K	773	FAD	C4X-C10-N10	2.65	120.36	116.48
2	J	773	FAD	C4X-C10-N1	-2.63	118.63	124.73
2	G	773	FAD	O2-C2-N3	2.61	123.72	118.65
2	E	773	FAD	C4-N3-C2	-2.61	120.82	125.64
2	E	773	FAD	C5X-C9A-N10	2.59	120.63	117.95
2	B	773	FAD	O4-C4-C4X	-2.56	119.80	126.60
2	J	773	FAD	O4-C4-C4X	-2.56	119.81	126.60
2	C	773	FAD	C4-N3-C2	-2.55	120.94	125.64
2	J	773	FAD	C4X-C4-N3	2.54	119.65	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	773	FAD	O2-C2-N3	2.53	123.57	118.65
2	F	773	FAD	C10-C4X-N5	-2.53	119.48	124.86
2	K	773	FAD	C4-N3-C2	-2.53	120.97	125.64
2	L	773	FAD	C4-C4X-N5	2.52	121.82	118.23
2	C	773	FAD	C10-N1-C2	2.49	121.88	116.90
2	A	773	FAD	O4-C4-C4X	-2.48	120.01	126.60
2	K	773	FAD	C4X-C4-N3	2.48	119.48	113.19
2	I	773	FAD	C5X-C9A-N10	2.47	120.50	117.95
2	J	773	FAD	C10-C4X-N5	-2.47	119.62	124.86
2	L	773	FAD	C5X-N5-C4X	2.44	122.14	118.07
2	C	773	FAD	C4X-C10-N1	-2.43	119.08	124.73
2	D	773	FAD	C4A-C5A-N7A	-2.43	106.86	109.40
2	E	773	FAD	C10-C4X-N5	-2.43	119.70	124.86
2	B	773	FAD	C4-C4X-C10	2.41	120.85	116.79
2	A	773	FAD	C9A-C5X-N5	-2.40	119.82	122.43
2	A	773	FAD	C4X-C4-N3	2.40	119.30	113.19
2	D	773	FAD	C4X-C10-N10	2.40	119.99	116.48
2	F	773	FAD	O4-C4-C4X	-2.40	120.24	126.60
2	H	773	FAD	O3B-C3B-C4B	-2.39	104.12	111.05
2	J	773	FAD	C4-C4X-C10	2.38	120.80	116.79
2	G	773	FAD	C5A-C6A-N6A	2.38	123.96	120.35
2	E	773	FAD	C9-C9A-N10	-2.34	118.68	121.84
2	H	773	FAD	C1'-N10-C9A	2.34	124.41	120.51
2	A	773	FAD	P-O3P-PA	-2.33	124.83	132.83
2	J	773	FAD	P-O3P-PA	-2.33	124.85	132.83
2	D	773	FAD	C4X-C10-N1	-2.32	119.34	124.73
2	C	773	FAD	C4X-C10-N10	2.32	119.87	116.48
2	E	773	FAD	O4-C4-C4X	-2.31	120.46	126.60
2	I	773	FAD	C4X-C4-N3	2.30	119.03	113.19
2	B	773	FAD	O4'-C4'-C5'	-2.30	104.75	109.92
2	C	773	FAD	C9A-C5X-N5	-2.30	119.93	122.43
2	G	773	FAD	C4X-C10-N1	-2.29	119.42	124.73
2	B	773	FAD	C4A-C5A-N7A	-2.29	107.01	109.40
2	B	773	FAD	C4X-C10-N10	2.28	119.81	116.48
2	K	773	FAD	O4-C4-C4X	-2.27	120.57	126.60
2	G	773	FAD	O2-C2-N1	-2.27	118.07	121.83
2	E	773	FAD	C4-C4X-N5	2.27	121.46	118.23
2	A	773	FAD	C4X-C10-N1	-2.26	119.49	124.73
2	F	773	FAD	C4X-C10-N10	2.25	119.77	116.48
2	C	773	FAD	C4A-C5A-N7A	-2.24	107.06	109.40
2	L	773	FAD	C4A-C5A-N7A	-2.24	107.07	109.40
2	A	773	FAD	C4-C4X-C10	2.22	120.52	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	773	FAD	O2-C2-N1	-2.18	118.22	121.83
2	E	773	FAD	C4X-C4-N3	2.17	118.71	113.19
2	D	773	FAD	C1B-N9A-C4A	-2.17	122.83	126.64
2	I	773	FAD	C10-C4X-N5	-2.15	120.29	124.86
2	K	773	FAD	C10-C4X-N5	-2.12	120.36	124.86
2	F	773	FAD	C9A-C5X-N5	-2.10	120.15	122.43
2	B	773	FAD	C6-C5X-C9A	2.10	121.91	118.94
2	E	773	FAD	C4X-C10-N10	2.10	119.55	116.48
2	A	773	FAD	C4X-C10-N10	2.08	119.53	116.48
2	C	773	FAD	C5X-C9A-N10	2.07	120.10	117.95
2	I	773	FAD	C3B-C2B-C1B	2.07	104.10	100.98
2	A	773	FAD	C1B-N9A-C4A	-2.07	123.01	126.64
2	A	773	FAD	C7M-C7-C8	2.06	124.96	120.74
2	B	773	FAD	C10-N1-C2	2.06	121.02	116.90
2	I	773	FAD	C4A-C5A-N7A	-2.05	107.26	109.40
2	A	773	FAD	C10-C4X-N5	-2.04	120.52	124.86
2	F	773	FAD	C4-C4X-C10	2.04	120.22	116.79
2	L	773	FAD	C5'-C4'-C3'	-2.03	108.27	112.20
2	H	773	FAD	C4X-C4-N3	2.02	118.31	113.19

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	773	FAD	O4B-C4B-C5B-O5B
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	O4B-C4B-C5B-O5B
2	C	773	FAD	N10-C1'-C2'-O2'
2	C	773	FAD	N10-C1'-C2'-C3'
2	E	773	FAD	O4B-C4B-C5B-O5B
2	E	773	FAD	C5'-O5'-P-O1P
2	F	773	FAD	O4B-C4B-C5B-O5B
2	G	773	FAD	O4'-C4'-C5'-O5'
2	G	773	FAD	C5'-O5'-P-O1P
2	J	773	FAD	O4B-C4B-C5B-O5B

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

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Mol	Chain	Res	Type	Atoms
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	A	773	FAD	C2'-C3'-C4'-C5'
2	K	773	FAD	C4B-C5B-O5B-PA
2	G	773	FAD	O4B-C4B-C5B-O5B
2	B	773	FAD	P-O3P-PA-O2A
2	F	773	FAD	P-O3P-PA-O1A
2	L	773	FAD	C4B-C5B-O5B-PA
2	E	773	FAD	C5B-O5B-PA-O2A
2	G	773	FAD	C3'-C4'-C5'-O5'
2	H	773	FAD	C3'-C4'-C5'-O5'
2	C	773	FAD	C4B-C5B-O5B-PA
2	D	773	FAD	N10-C1'-C2'-O2'
2	F	773	FAD	C2'-C1'-N10-C10

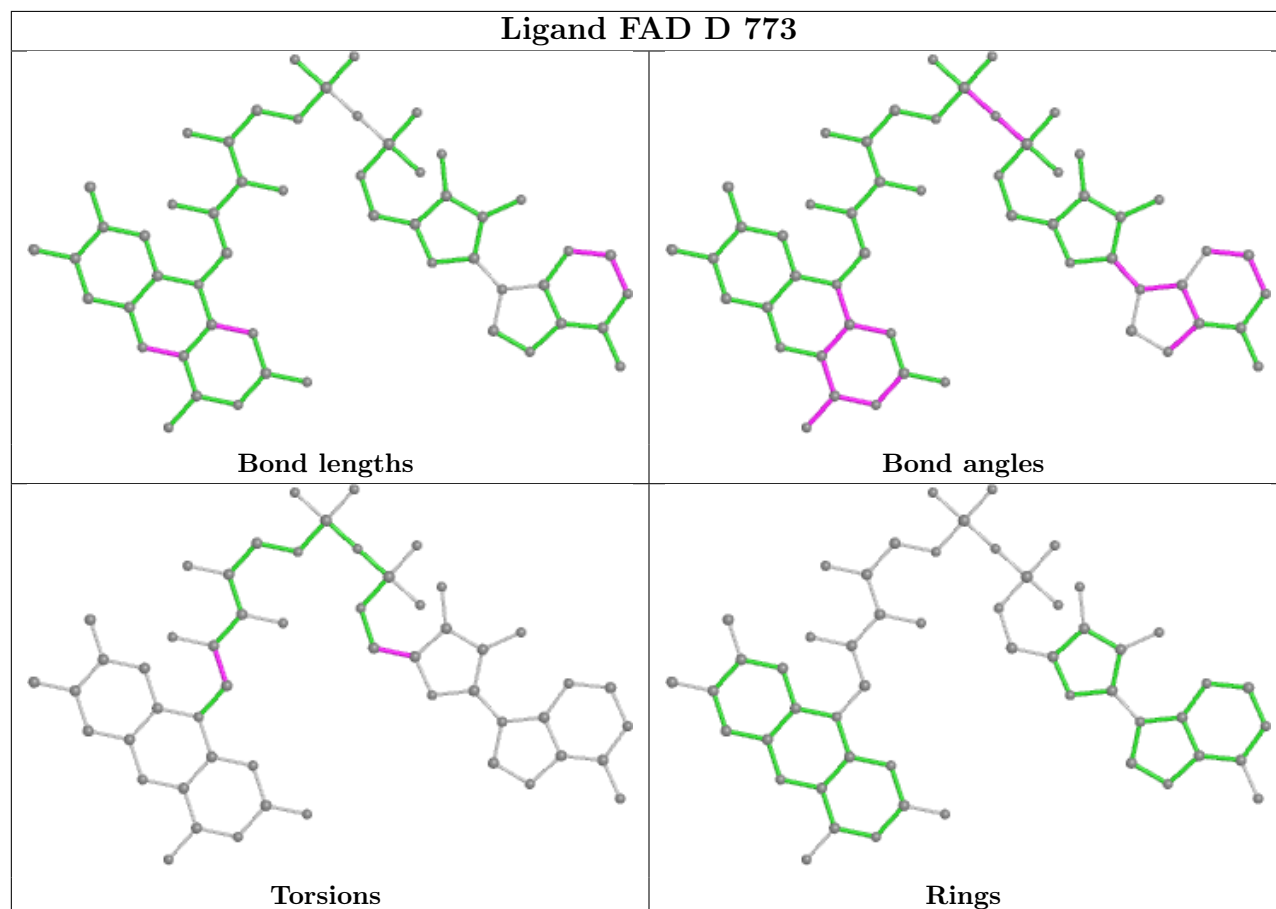
There are no ring outliers.

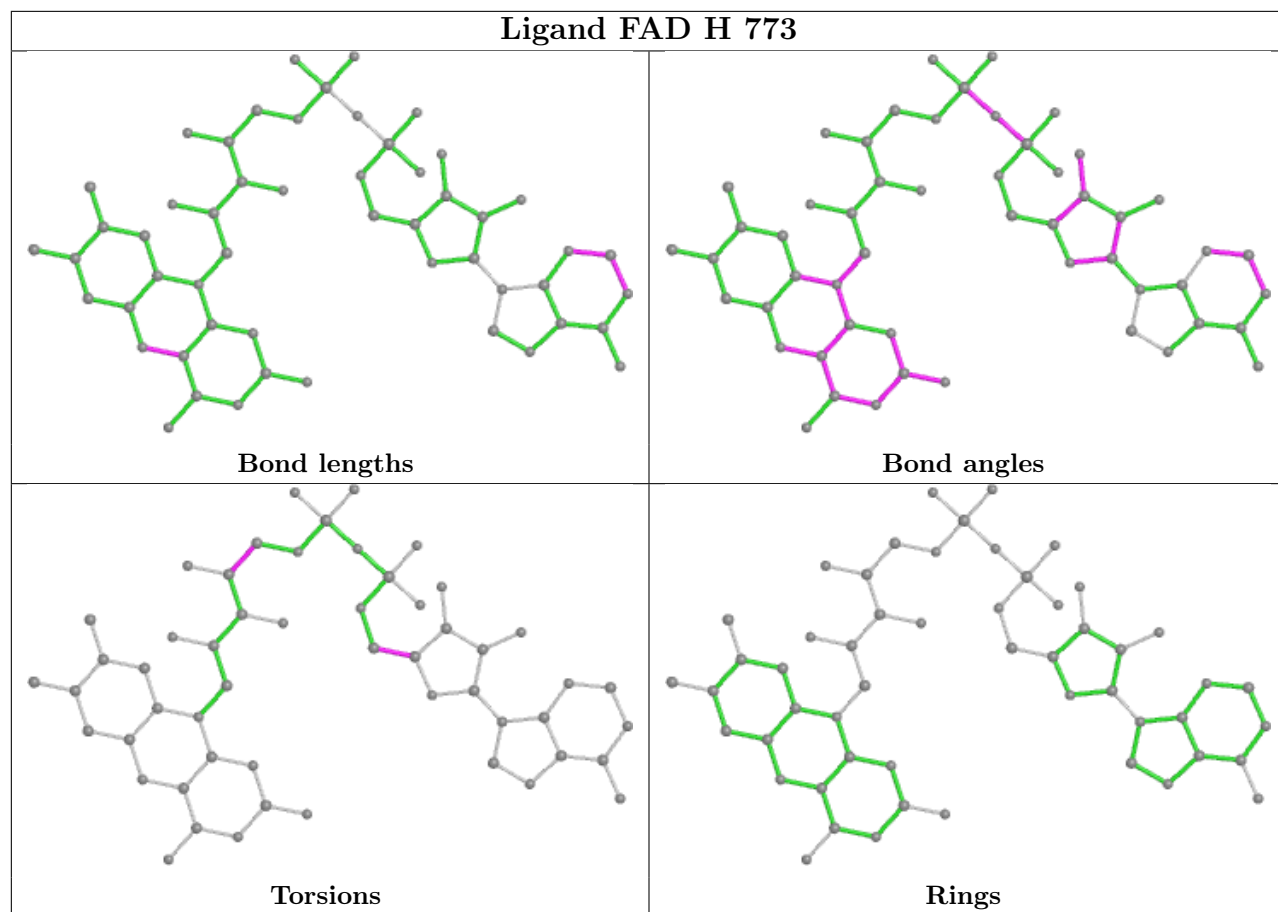
12 monomers are involved in 76 short contacts:

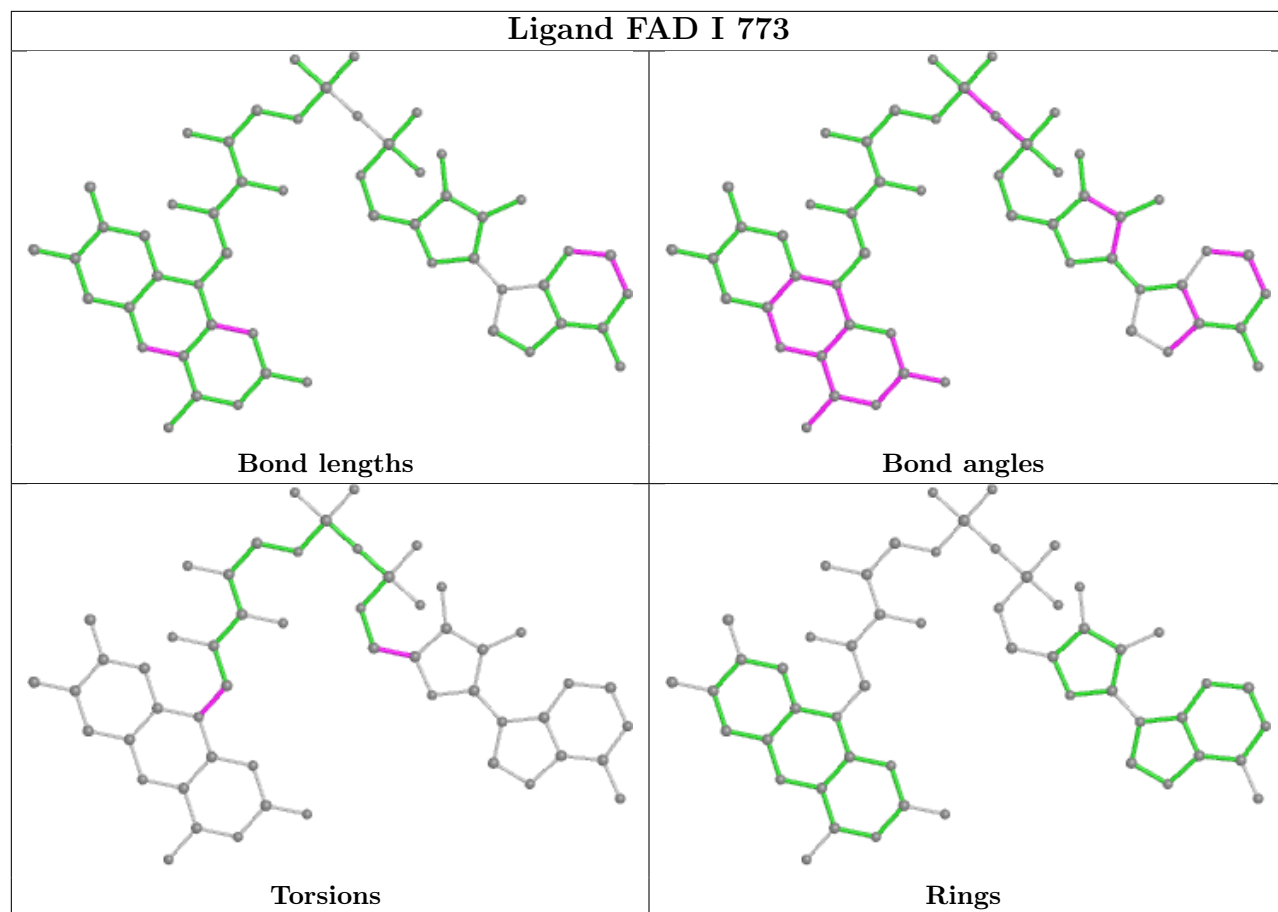
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	773	FAD	12	0
2	H	773	FAD	7	0
2	I	773	FAD	5	0
2	G	773	FAD	4	0
2	J	773	FAD	6	0
2	F	773	FAD	5	0
2	K	773	FAD	7	0
2	L	773	FAD	5	0
2	C	773	FAD	6	0
2	E	773	FAD	8	0
2	A	773	FAD	6	0
2	B	773	FAD	5	0

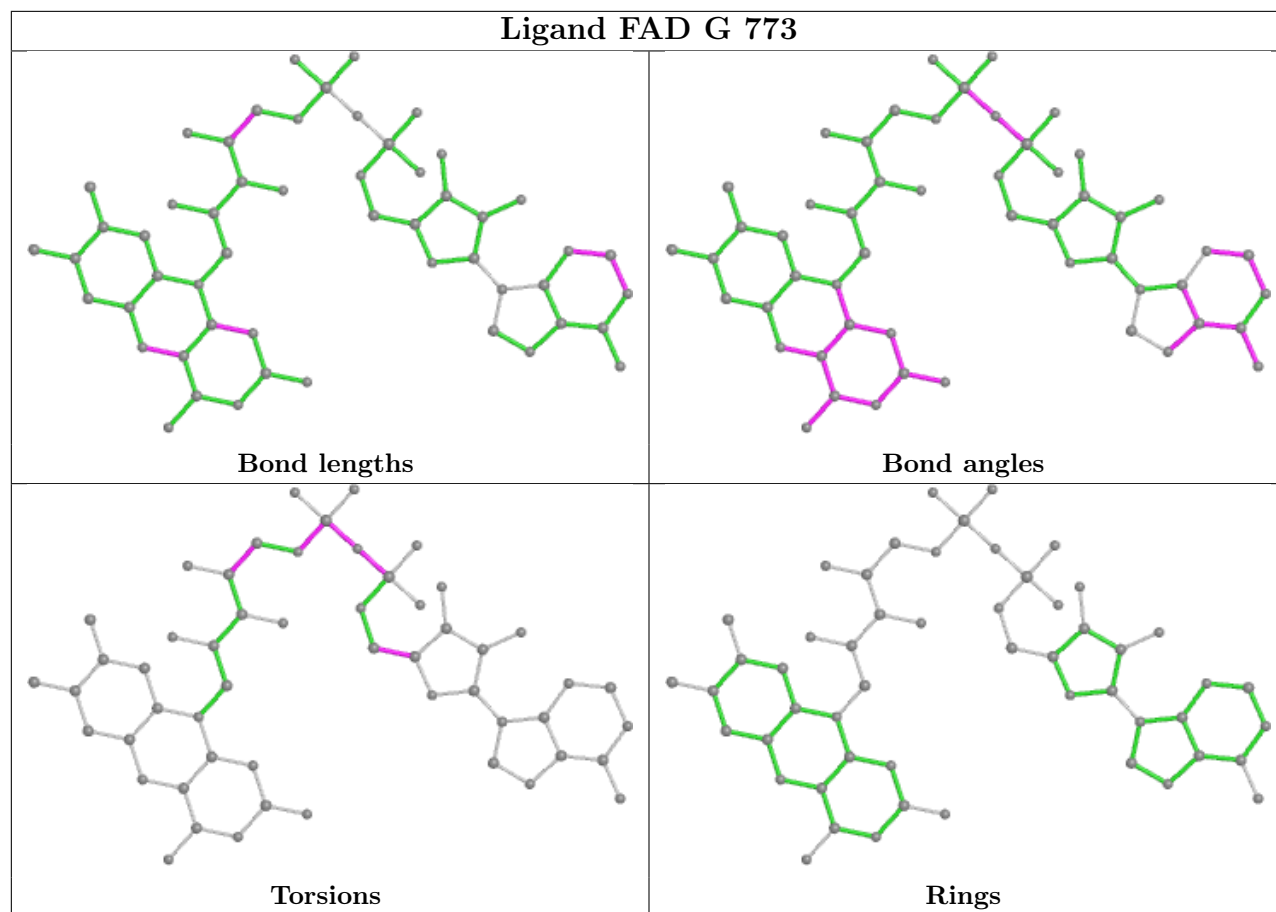
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

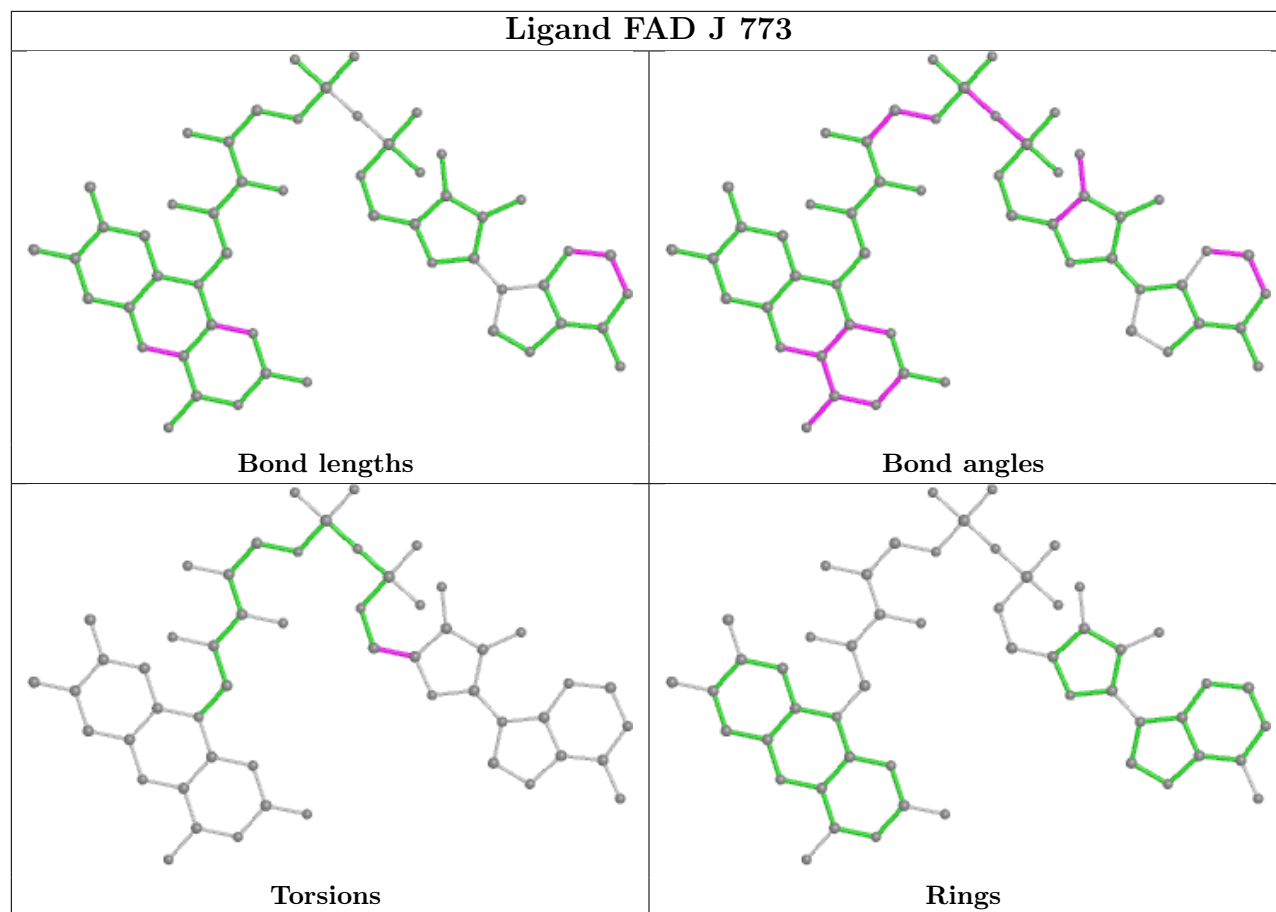
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

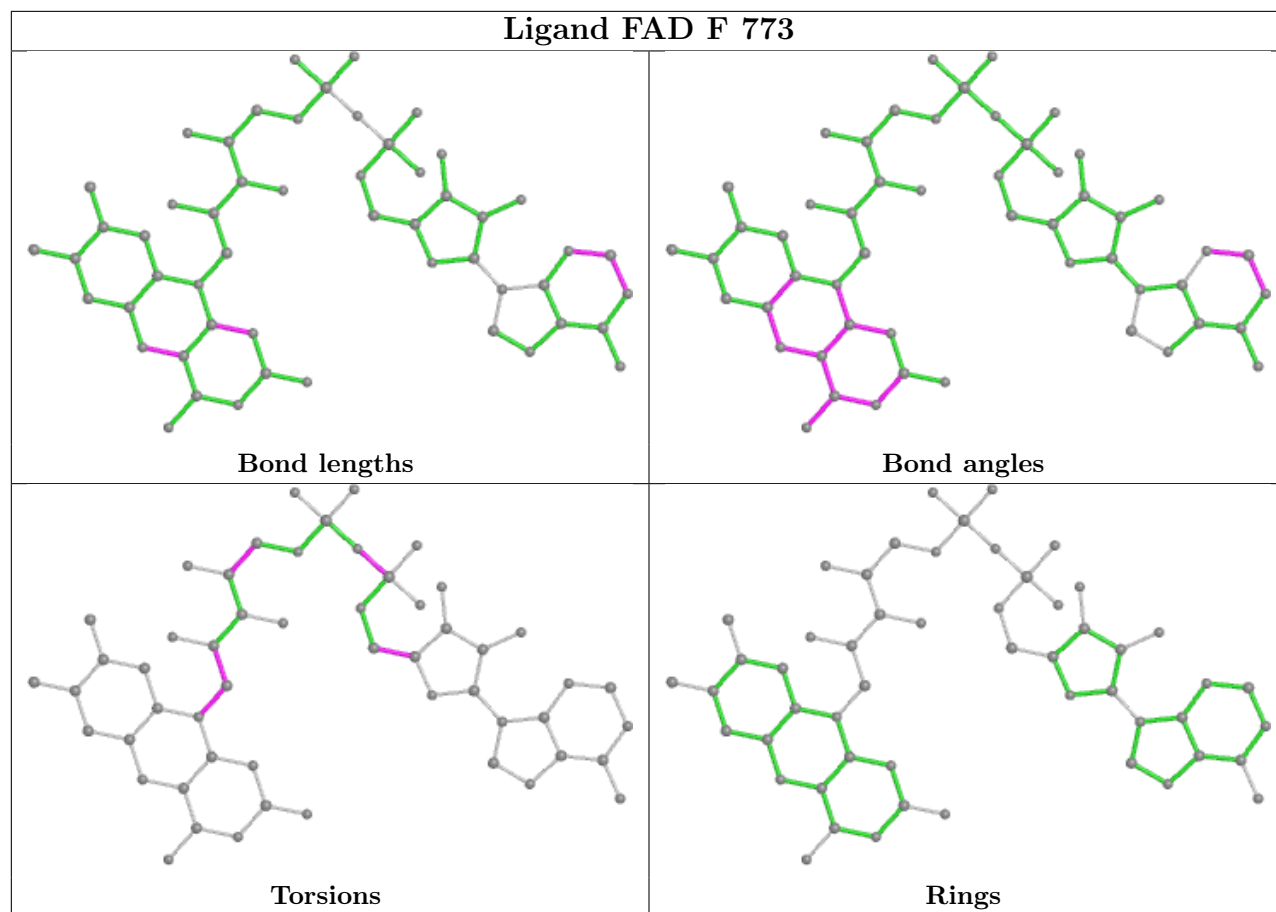


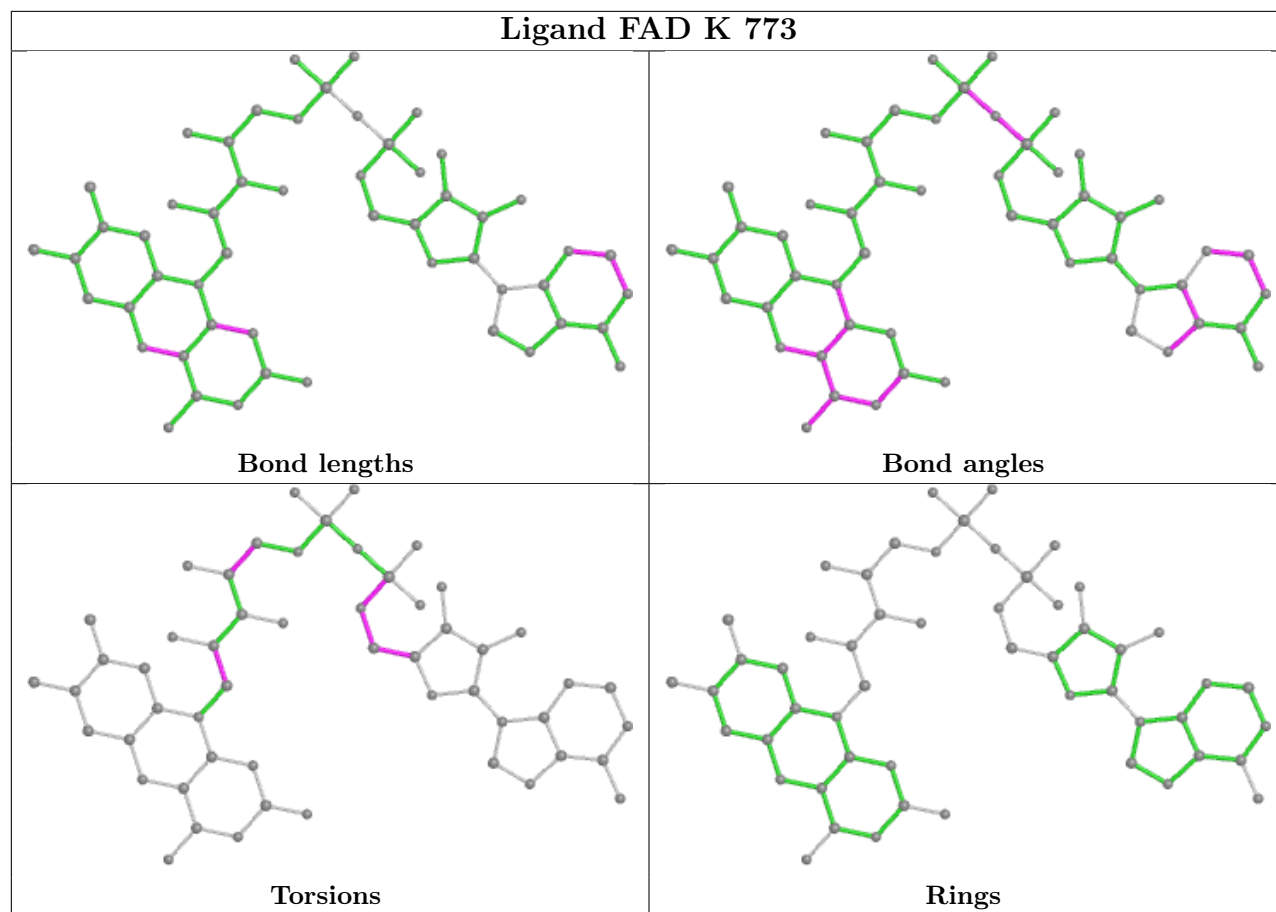


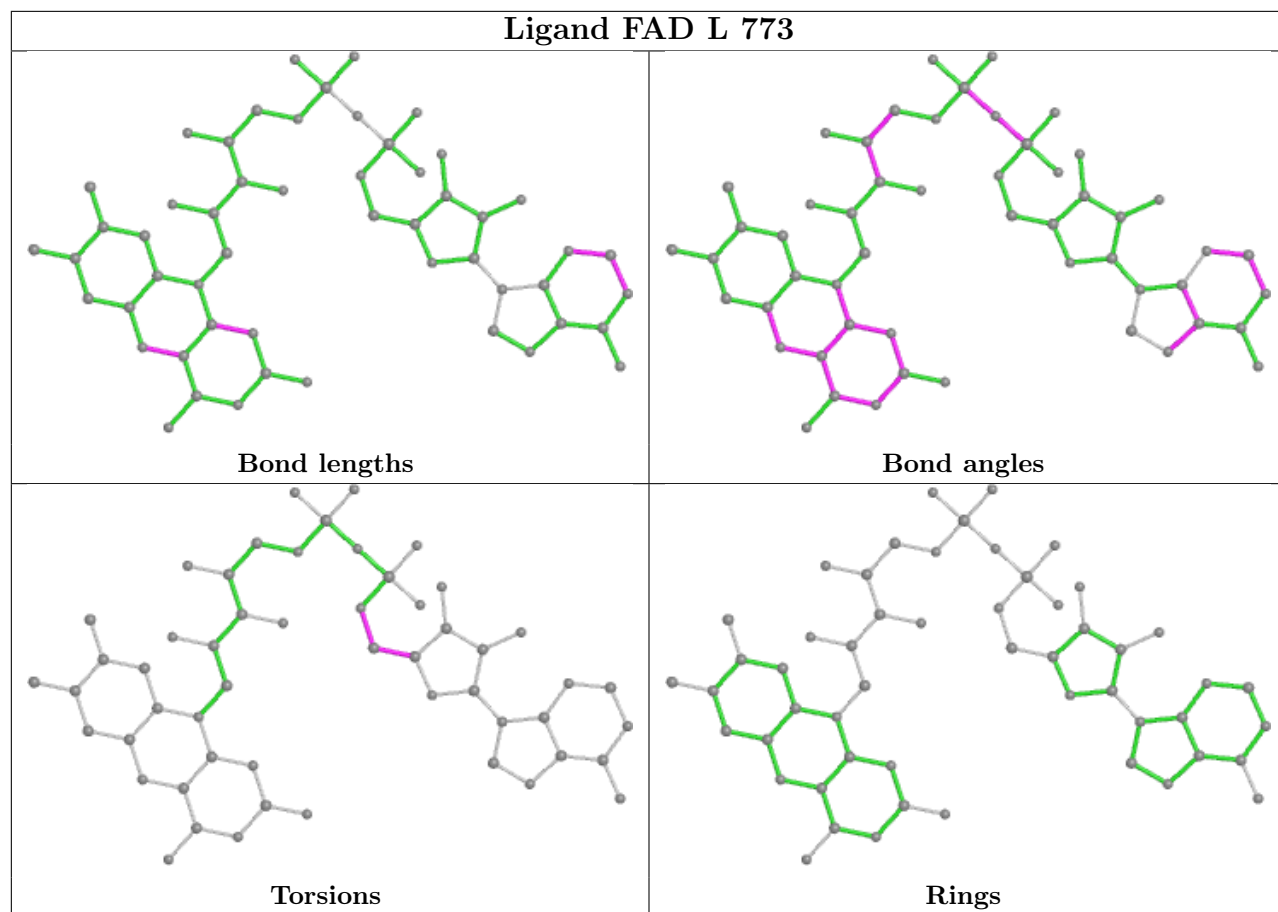


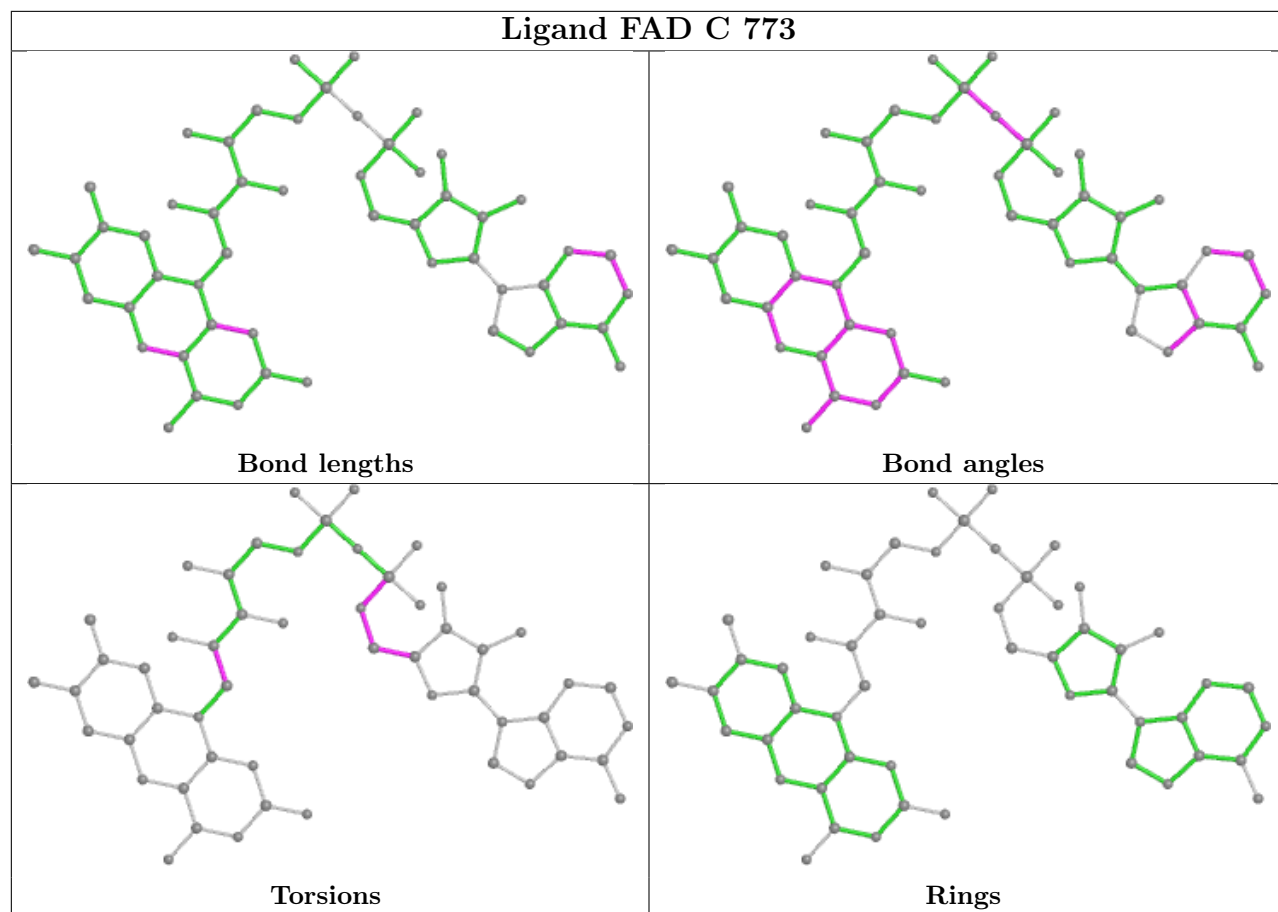


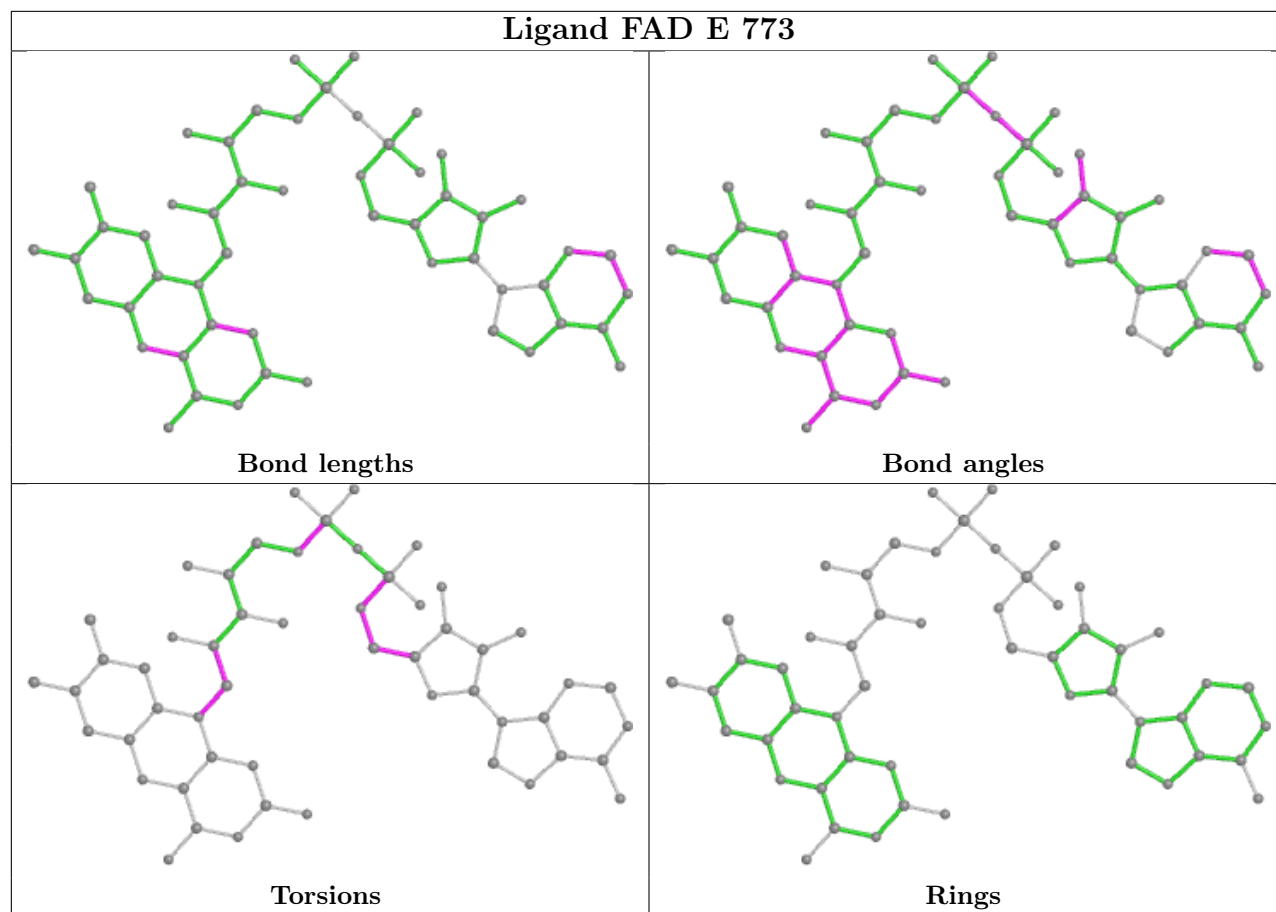


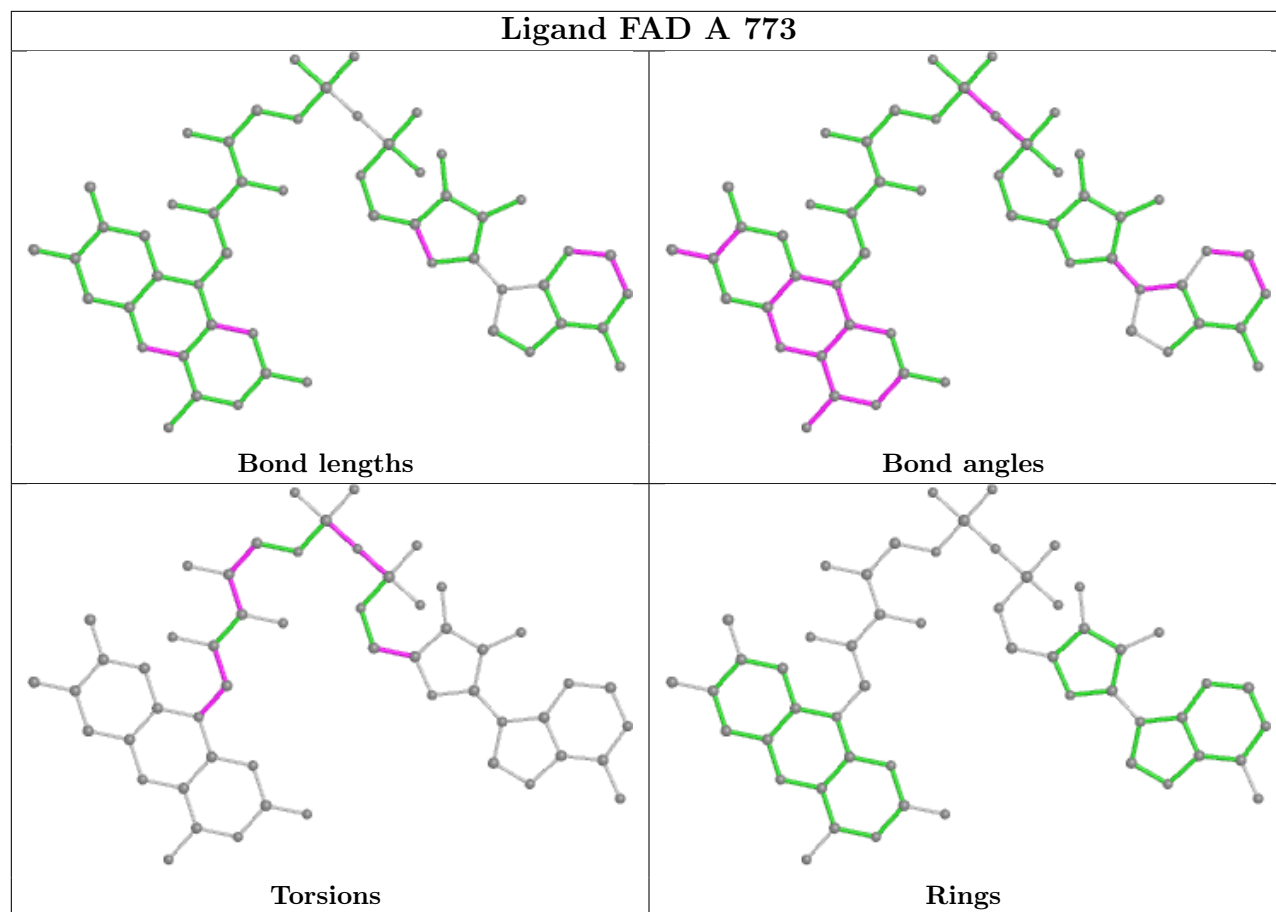


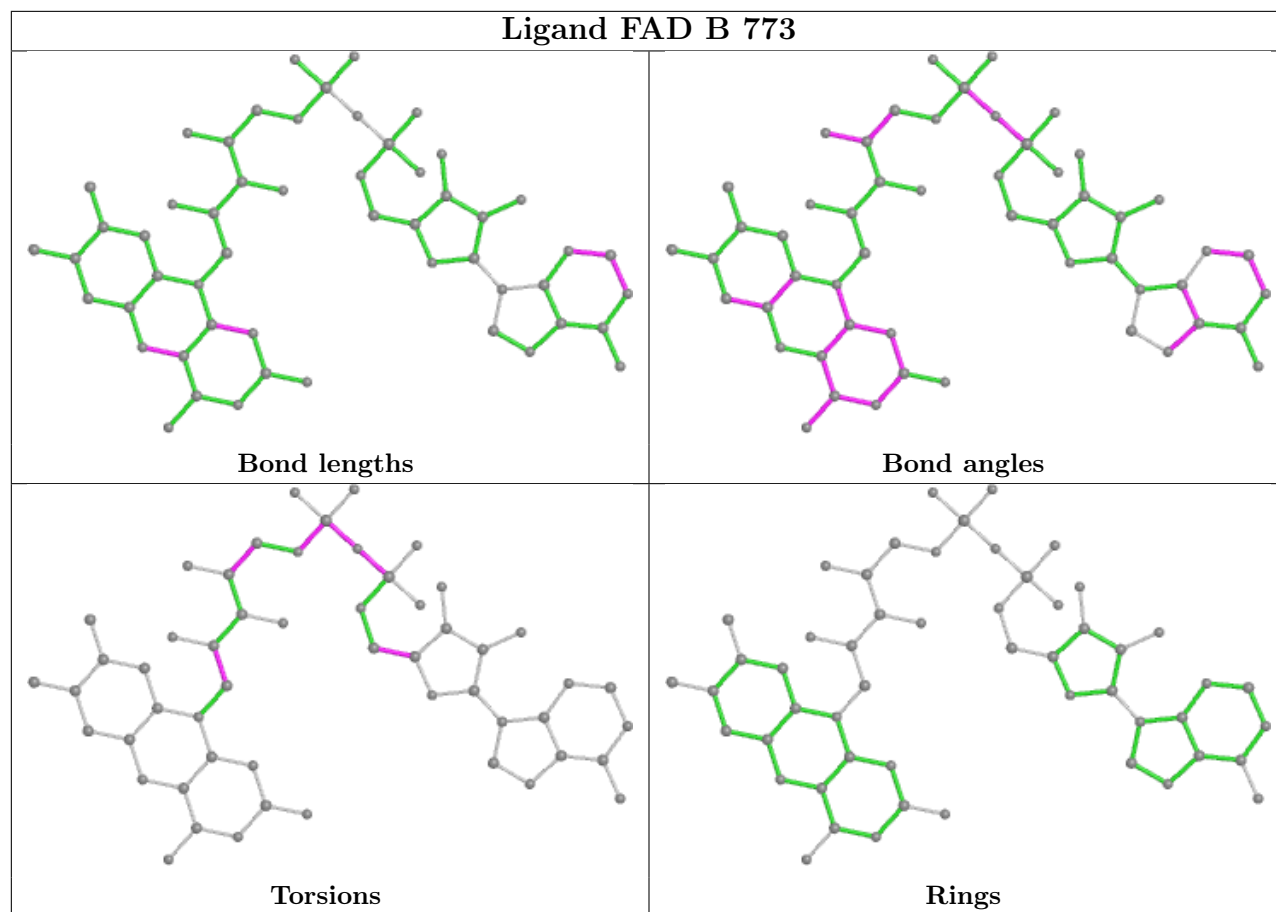












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	521/521 (100%)	-0.76	2 (0%) 92 79	9, 23, 38, 51	0
1	B	521/521 (100%)	-0.75	4 (0%) 86 65	12, 23, 35, 53	0
1	C	521/521 (100%)	-0.74	4 (0%) 86 65	11, 24, 37, 53	0
1	D	521/521 (100%)	-0.72	3 (0%) 89 72	9, 23, 40, 53	0
1	E	521/521 (100%)	-0.72	4 (0%) 86 65	10, 25, 39, 50	0
1	F	521/521 (100%)	-0.75	3 (0%) 89 72	11, 23, 38, 51	0
1	G	521/521 (100%)	-0.74	5 (0%) 82 59	13, 24, 37, 51	0
1	H	521/521 (100%)	-0.70	3 (0%) 89 72	12, 26, 41, 50	0
1	I	521/521 (100%)	-0.64	4 (0%) 86 65	15, 28, 44, 55	0
1	J	521/521 (100%)	-0.66	4 (0%) 86 65	16, 28, 42, 54	0
1	K	521/521 (100%)	-0.56	6 (1%) 79 53	14, 31, 46, 57	0
1	L	521/521 (100%)	-0.45	6 (1%) 79 53	20, 35, 49, 55	0
All	All	6252/6252 (100%)	-0.68	48 (0%) 86 65	9, 26, 43, 57	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	227	SER	6.2
1	I	226	SER	6.0
1	I	225	ASN	4.6
1	J	227	SER	4.5
1	F	226	SER	4.5
1	A	227	SER	4.1
1	K	226	SER	4.0
1	F	225	ASN	3.8
1	B	226	SER	3.7
1	D	226	SER	3.7
1	D	227	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	226	SER	3.5
1	E	226	SER	3.4
1	H	226	SER	3.3
1	H	225	ASN	3.1
1	B	227	SER	3.0
1	D	225	ASN	3.0
1	H	227	SER	3.0
1	C	226	SER	2.8
1	L	132	ASP	2.8
1	K	132	ASP	2.8
1	E	227	SER	2.8
1	J	521	ALA	2.8
1	B	520	ALA	2.7
1	K	426	GLY	2.7
1	E	521	ALA	2.7
1	C	378	SER	2.6
1	E	225	ASN	2.6
1	G	226	SER	2.6
1	C	225	ASN	2.5
1	K	225	ASN	2.5
1	K	227	SER	2.5
1	L	225	ASN	2.5
1	I	521	ALA	2.5
1	G	228	GLY	2.4
1	L	226	SER	2.4
1	G	207	ASN	2.3
1	C	227	SER	2.3
1	B	225	ASN	2.2
1	A	225	ASN	2.2
1	L	428	ASP	2.2
1	F	227	SER	2.1
1	I	378	SER	2.1
1	L	123	SER	2.1
1	J	378	SER	2.1
1	K	378	SER	2.1
1	L	139	ASP	2.1
1	G	225	ASN	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

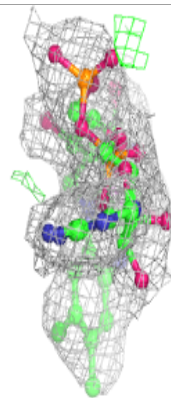
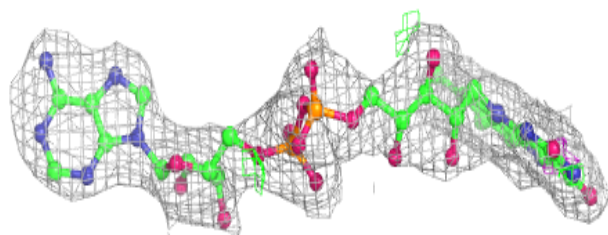
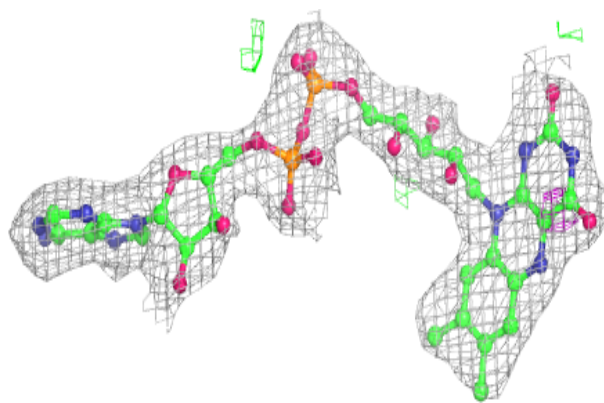
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	E	773	53/53	0.97	0.10	9,14,17,18	0
2	FAD	I	773	53/53	0.97	0.10	11,14,18,20	0
2	FAD	J	773	53/53	0.97	0.11	15,18,21,22	0
2	FAD	L	773	53/53	0.97	0.11	15,22,26,27	0
2	FAD	A	773	53/53	0.98	0.09	7,11,13,15	0
2	FAD	F	773	53/53	0.98	0.09	7,15,20,22	0
2	FAD	G	773	53/53	0.98	0.10	5,12,14,15	0
2	FAD	H	773	53/53	0.98	0.10	3,11,14,17	0
2	FAD	B	773	53/53	0.98	0.10	6,11,16,17	0
2	FAD	C	773	53/53	0.98	0.09	7,13,17,19	0
2	FAD	K	773	53/53	0.98	0.09	11,17,20,21	0
2	FAD	D	773	53/53	0.98	0.09	7,9,11,13	0

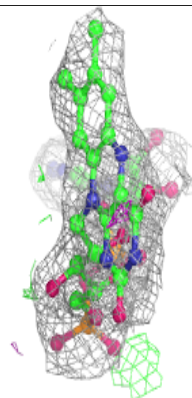
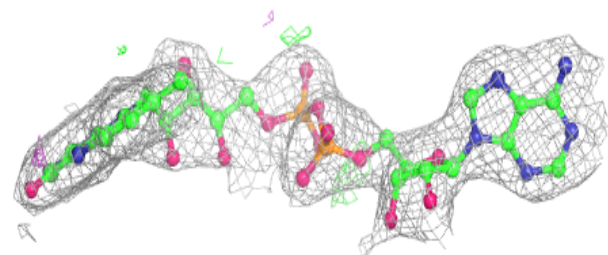
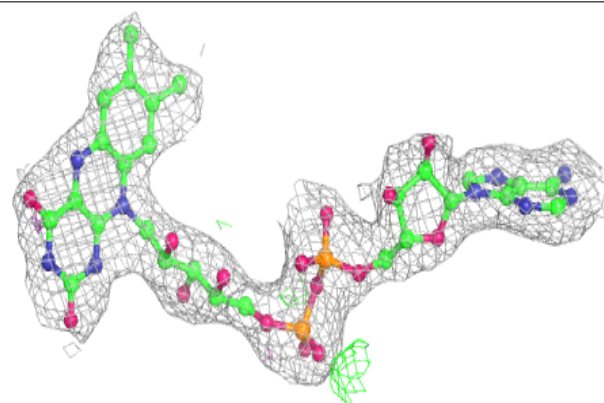
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

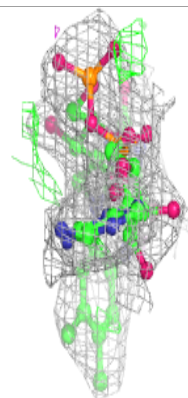
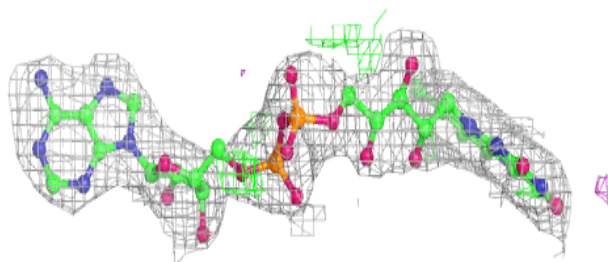
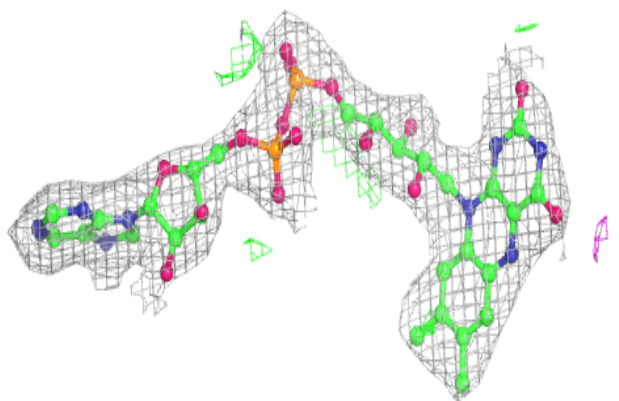
**Electron density around FAD I 773:**

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

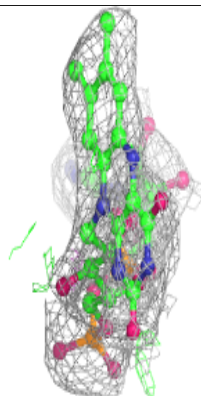
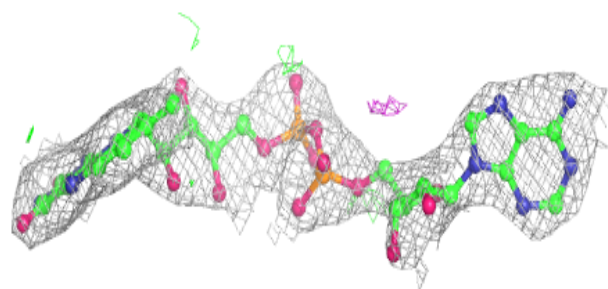
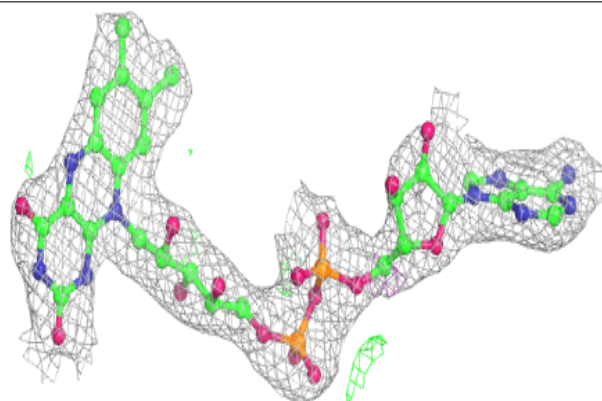


Electron density around FAD J 773:

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

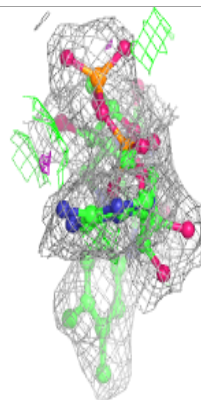
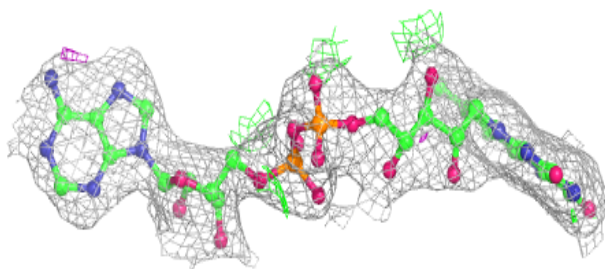
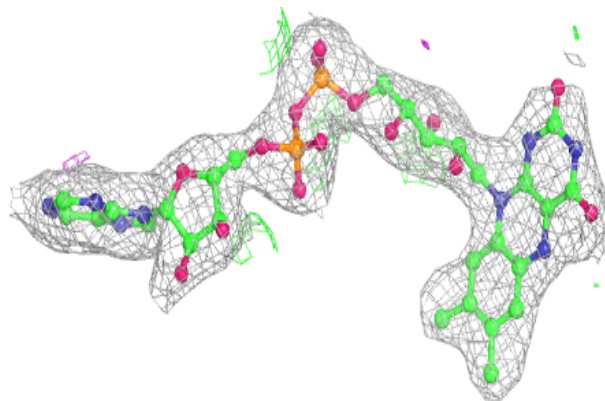
**Electron density around FAD L 773:**

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

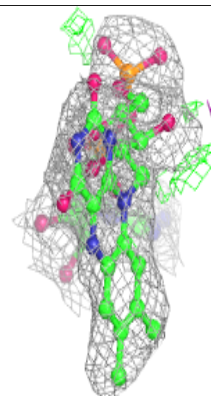
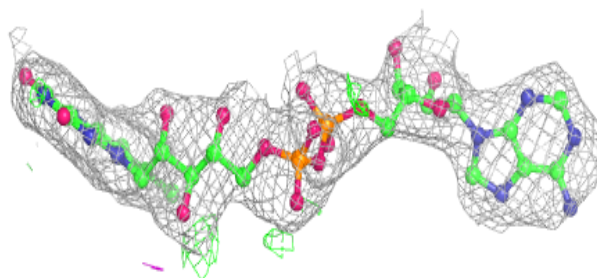
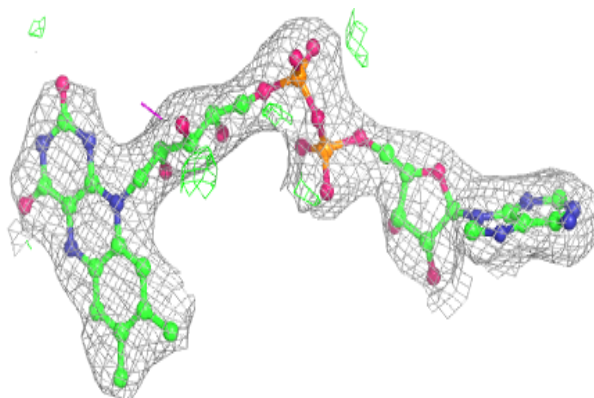


Electron density around FAD A 773:

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

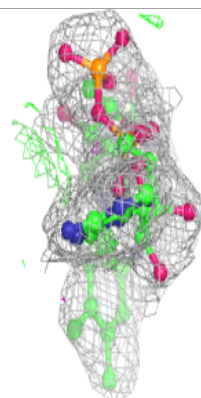
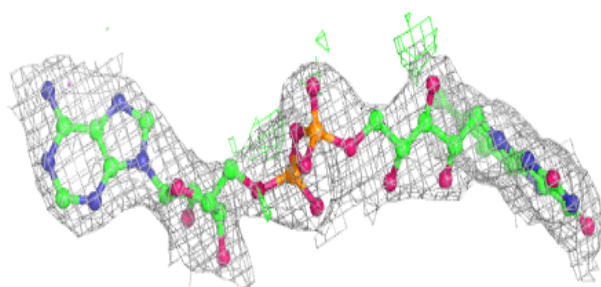
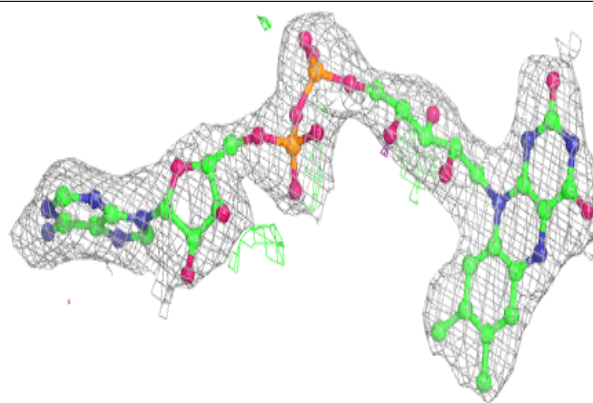
**Electron density around FAD F 773:**

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

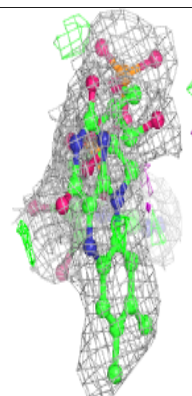
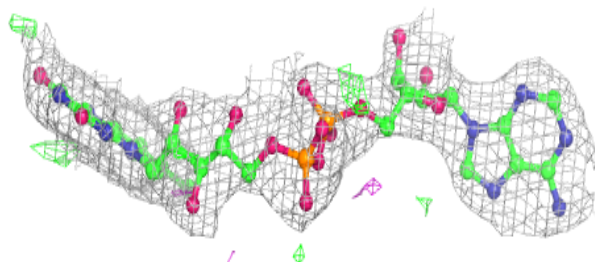
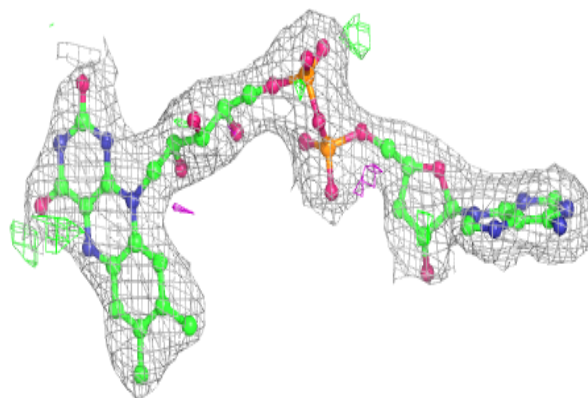


Electron density around FAD G 773:

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

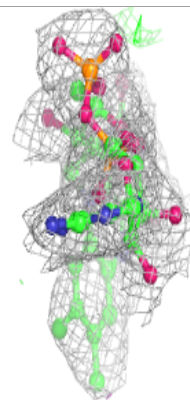
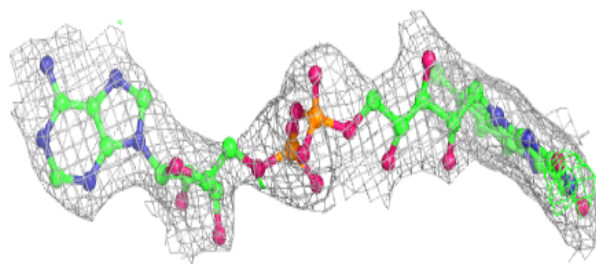
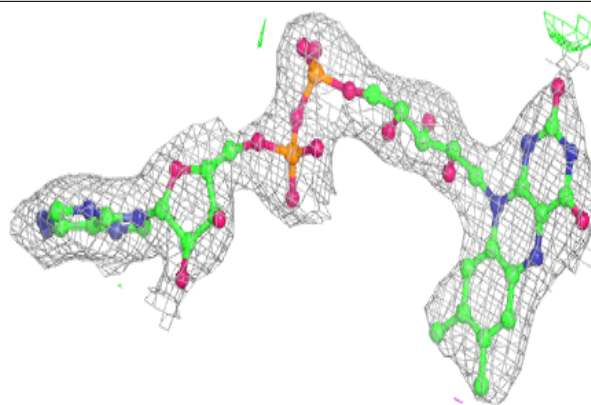
**Electron density around FAD H 773:**

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

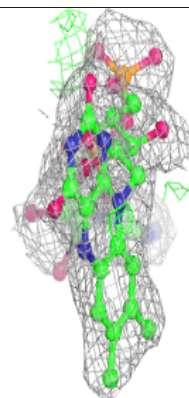
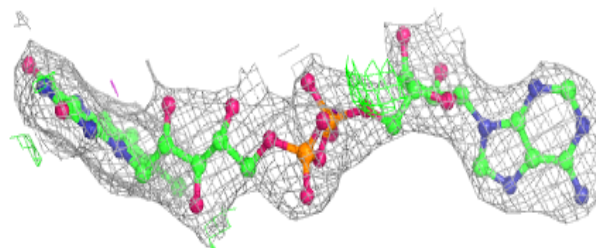
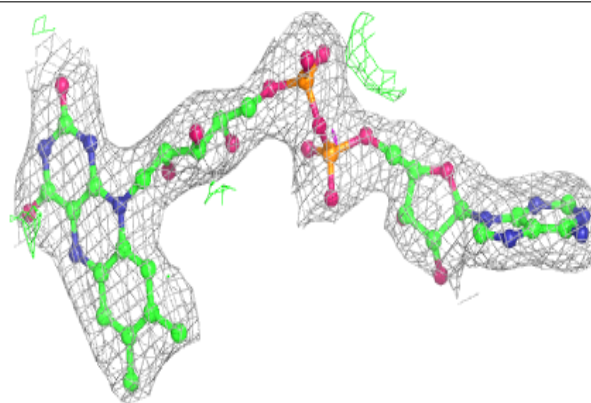


Electron density around FAD B 773:

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

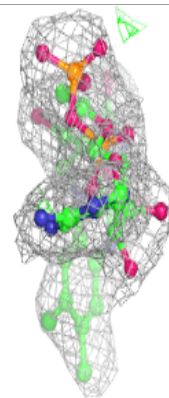
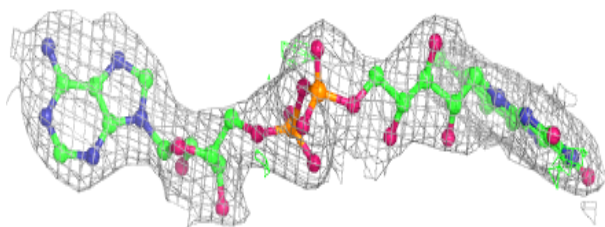
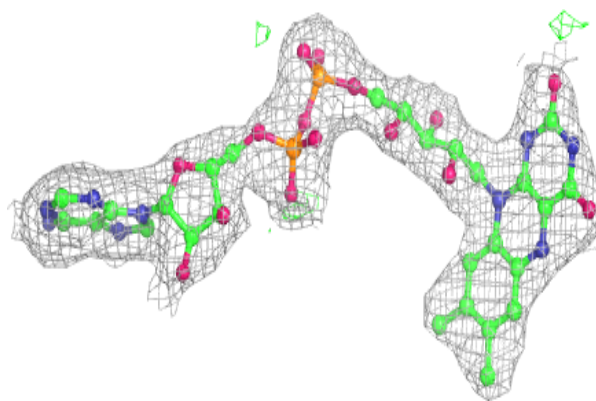
**Electron density around FAD C 773:**

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

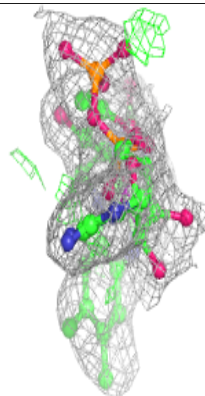
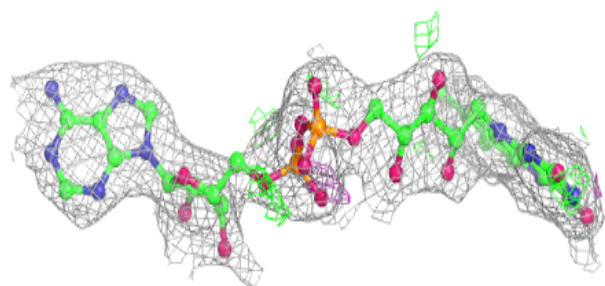
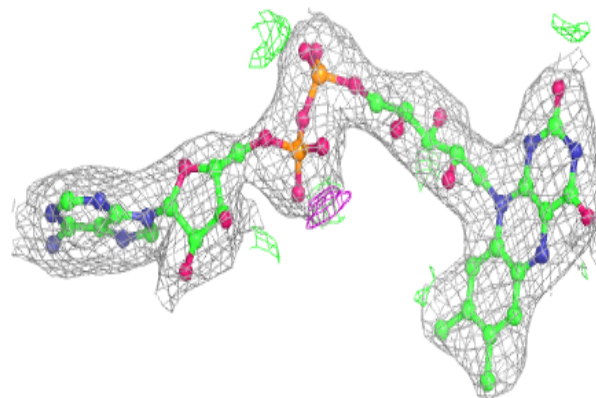


Electron density around FAD K 773:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.