Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 10:04 AM JST

PDB ID	:	6LLC
Title	:	Discovery of A Dual Inhibitor of NQO1 and GSTP1 for Treating Malignant Glioblastoma
Authors	:	Ye, K.; Li, H.
Deposited on	:	2019-12-23
Resolution	:	2.50 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:

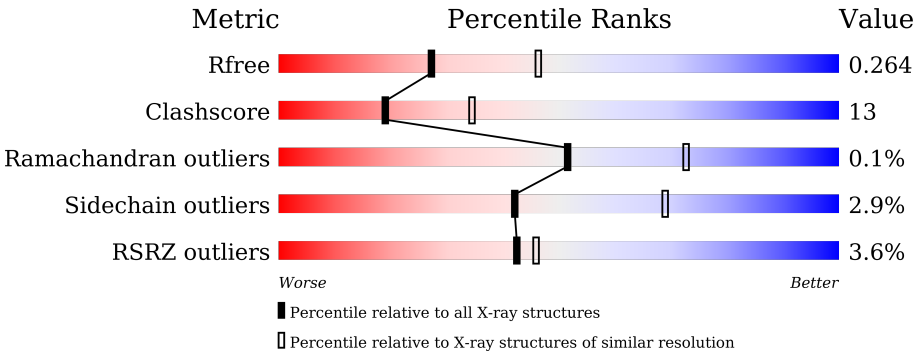
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	273	79% 19%
1	B	273	4% 70% 27%
1	C	273	3% 73% 25%
1	D	273	3% 76% 22%
1	E	273	2% 75% 23%
1	F	273	3% 69% 29%

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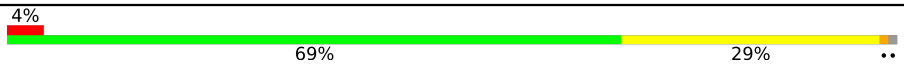
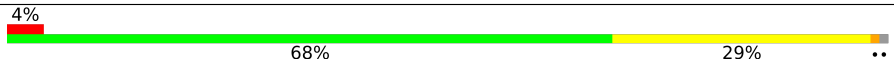
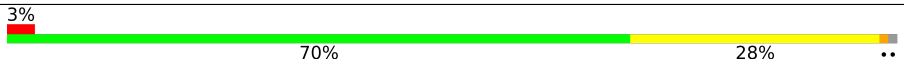
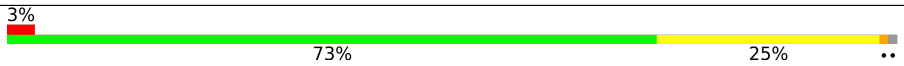
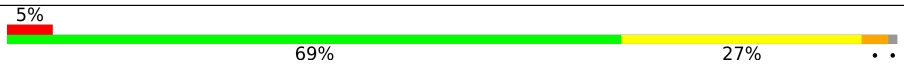
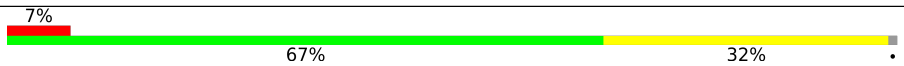
Mol	Chain	Length	Quality of chain
1	G	273	
1	H	273	
1	I	273	
1	J	273	
1	K	273	
1	L	273	

2 Entry composition (i)

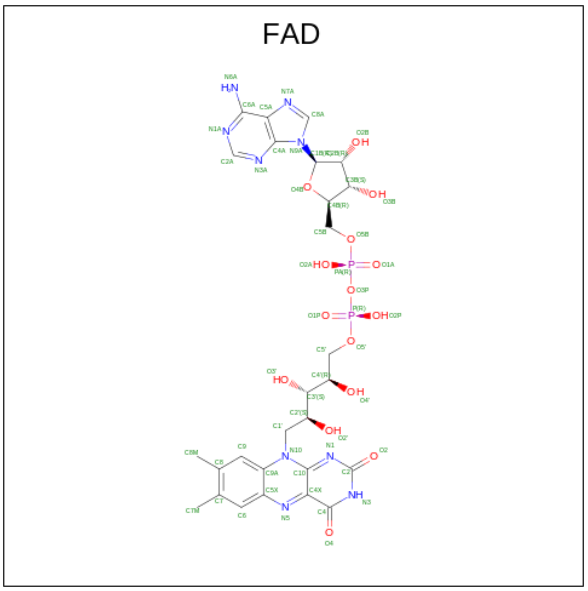
There are 5 unique types of molecules in this entry. The entry contains 27057 atoms, of which 70 are hydrogens and 0 are deuteriums.

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 NAD(P)H dehydrogenase [quinone] 1.

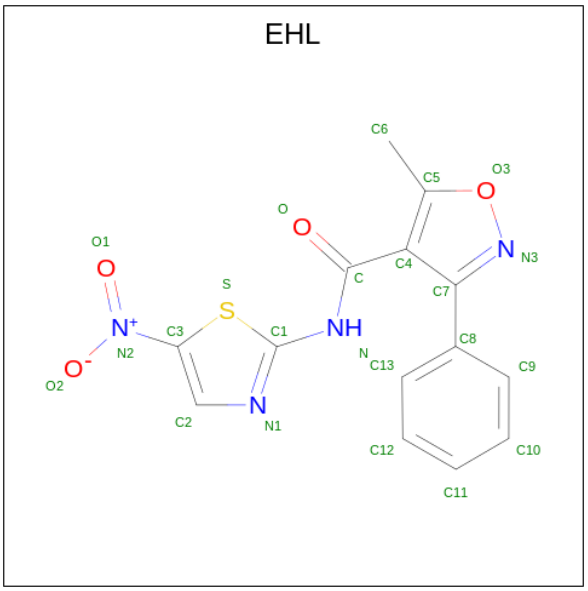
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2167	1409	364	387	7			
1	B	271	Total	C	N	O	S	0	0	0
			2158	1403	362	386	7			
1	C	271	Total	C	N	O	S	0	0	0
			2158	1403	362	386	7			
1	D	272	Total	C	N	O	S	0	0	0
			2167	1409	364	387	7			
1	E	271	Total	C	N	O	S	0	0	0
			2158	1403	362	386	7			
1	F	271	Total	C	N	O	S	0	0	0
			2158	1403	362	386	7			
1	G	270	Total	C	N	O	S	0	0	0
			2154	1401	361	385	7			
1	H	270	Total	C	N	O	S	0	0	0
			2154	1401	361	385	7			
1	I	270	Total	C	N	O	S	0	0	0
			2154	1401	361	385	7			
1	J	270	Total	C	N	O	S	0	0	0
			2154	1401	361	385	7			
1	K	271	Total	C	N	O	S	0	0	0
			2158	1403	362	386	7			
1	L	271	Total	C	N	O	S	0	0	0
			2158	1403	362	386	7			

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



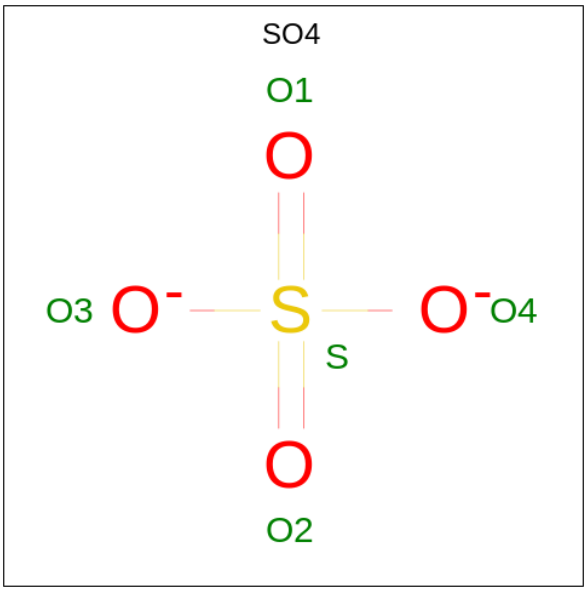
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	53	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	53	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	53	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	53	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	53	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	53	0
			53	27	9	15	2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

- Molecule 3 is 5-methyl-N-(5-nitro-1,3-thiazol-2-yl)-3-phenyl-1,2-oxazole-4-carboxamide (three-letter code: EHL) (formula: $C_{14}H_{10}N_4O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O S 33 14 10 4 4 1	33	0
3	B	1	Total C H N O S 33 14 10 4 4 1	33	0
3	D	1	Total C N O S 23 14 4 4 1	23	0
3	E	1	Total C H N O S 33 14 10 4 4 1	33	0
3	H	1	Total C H N O S 33 14 10 4 4 1	33	0
3	I	1	Total C H N O S 33 14 10 4 4 1	33	0
3	J	1	Total C H N O S 33 14 10 4 4 1	33	0
3	L	1	Total C H N O S 33 14 10 4 4 1	33	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	40	Total O 40 40	0	0
5	B	16	Total O 16 16	0	0
5	C	31	Total O 31 31	0	0
5	D	40	Total O 40 40	0	0
5	E	27	Total O 27 27	0	0
5	F	16	Total O 16 16	0	0
5	G	13	Total O 13 13	0	0
5	I	19	Total O 19 19	0	0

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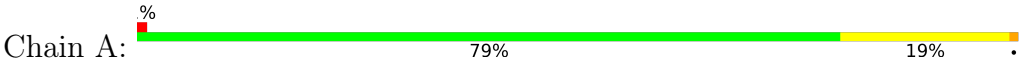
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	18	Total O 18 18	0	0
5	K	14	Total O 14 14	0	0
5	L	15	Total O 15 15	0	0

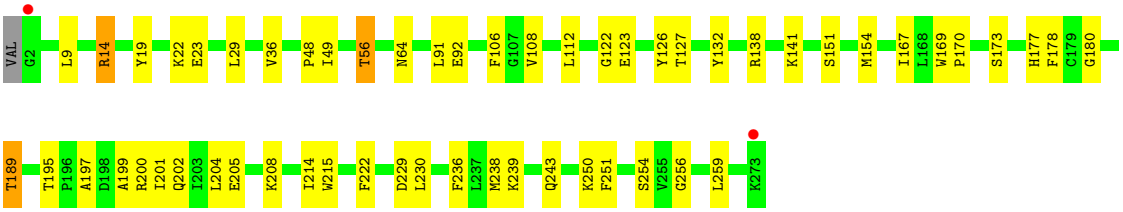
3 Residue-property plots (i)

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: NAD(P)H dehydrogenase [quinone] 1

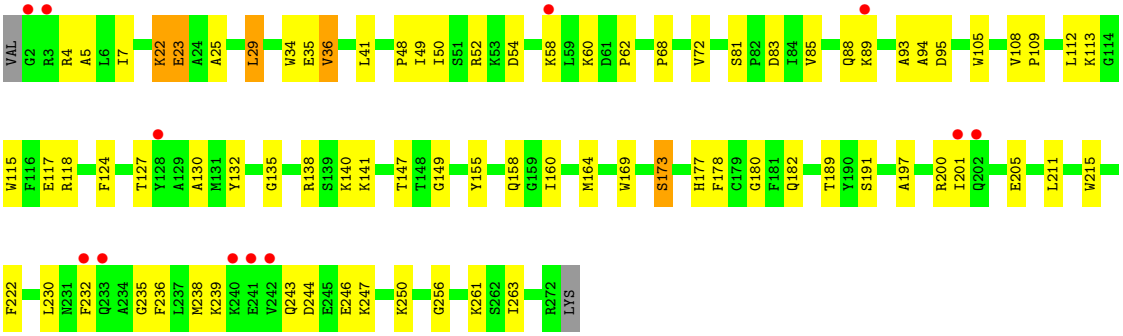
Chain A:





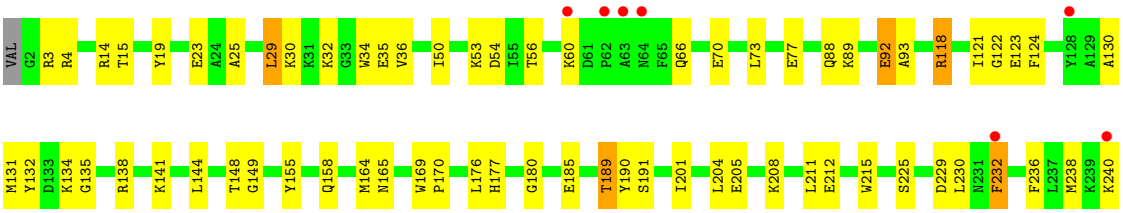
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

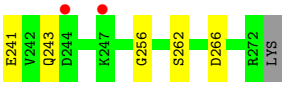
Chain B:



• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

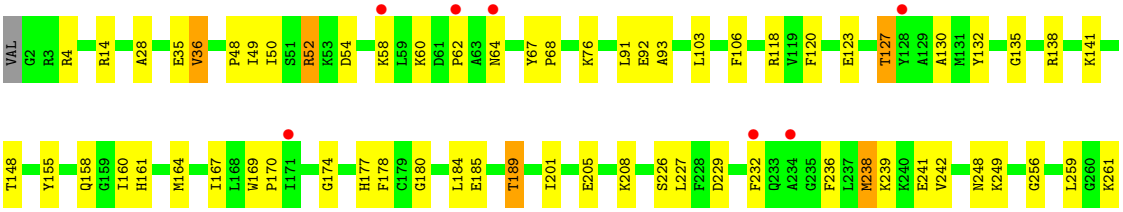
Chain C:





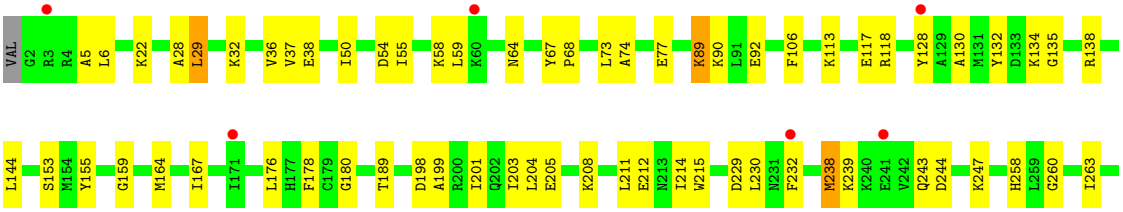
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain D:



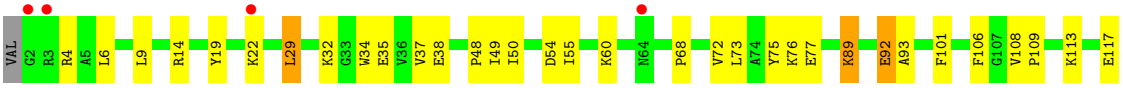
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

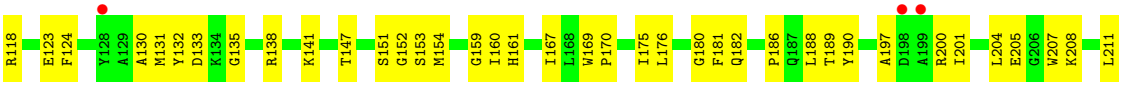
Chain E:

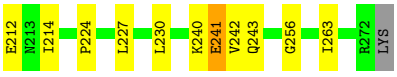


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain F:

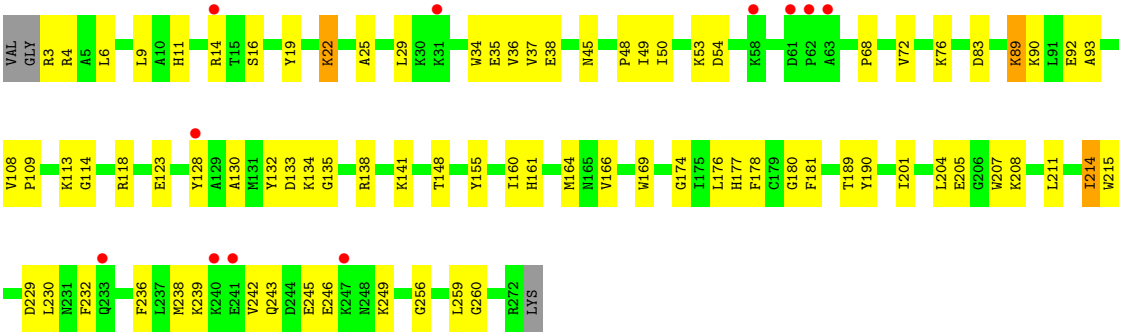






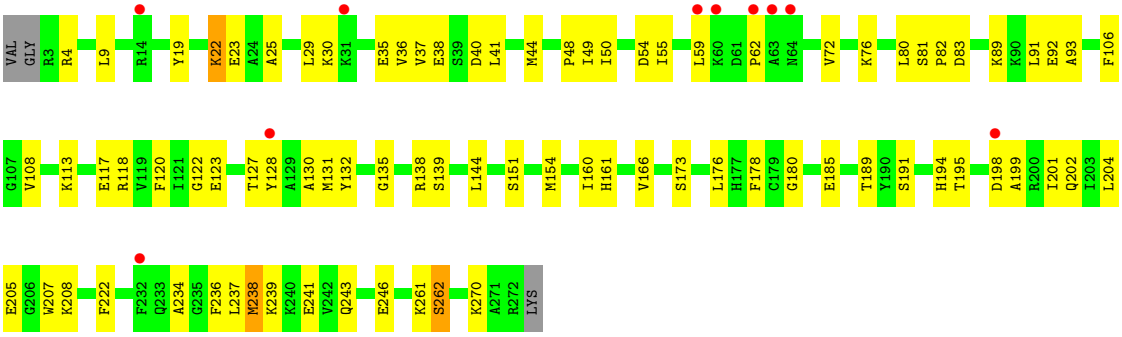
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain G:



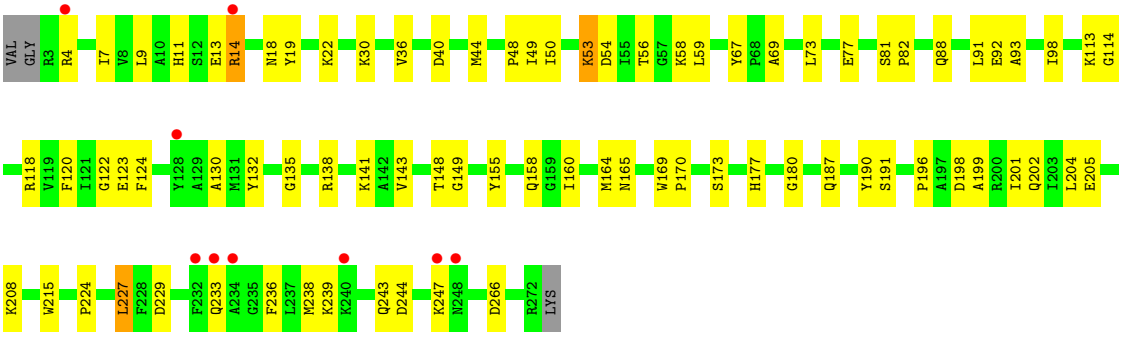
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain H:



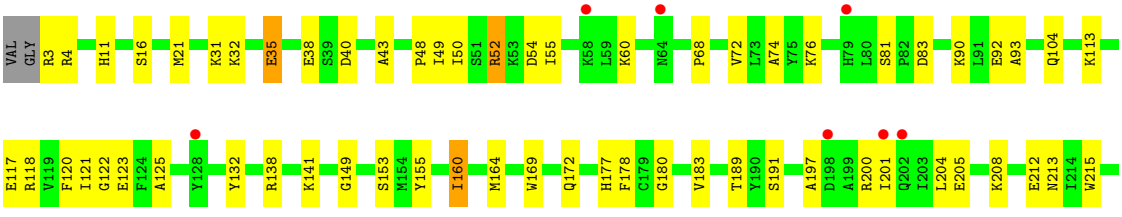
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain I:

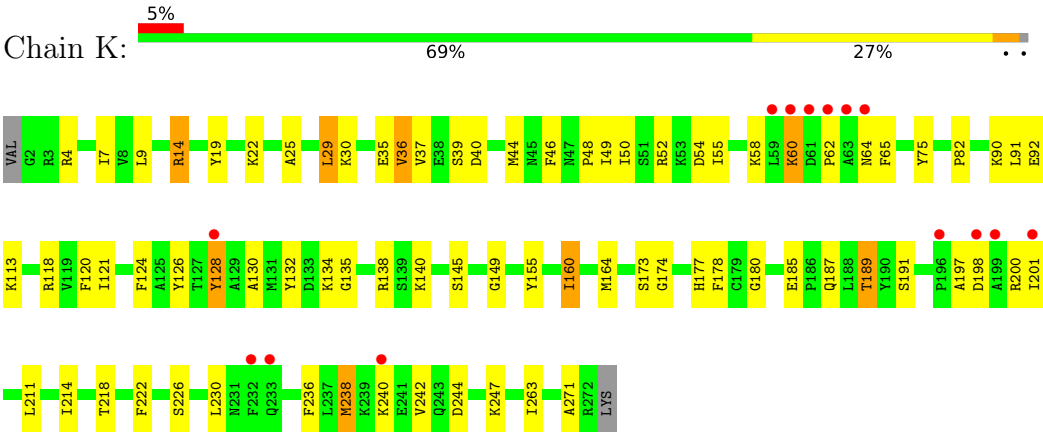


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

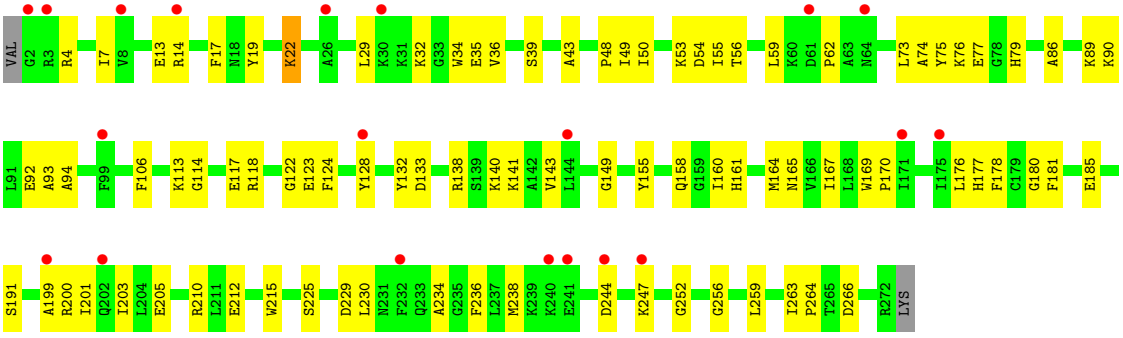
Chain J:



• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	147.88Å 147.88Å 209.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.50 29.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.58-2.50) 99.8 (29.58-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.222 , 0.265 0.222 , 0.264	Depositor DCC
R_{free} test set	2005 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27057	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EHL, 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	0.51	0/2225	0.61	0/3005
1	B	0.46	0/2216	0.57	0/2994
1	C	0.47	0/2216	0.59	1/2994 (0.0%)
1	D	0.52	0/2225	0.64	0/3005
1	E	0.47	0/2216	0.58	0/2994
1	F	0.45	0/2216	0.55	0/2994
1	G	0.45	0/2212	0.58	0/2989
1	H	0.47	0/2212	0.58	0/2989
1	I	0.43	0/2212	0.56	0/2989
1	J	0.44	0/2212	0.57	0/2989
1	K	0.43	0/2216	0.57	0/2994
1	L	0.43	0/2216	0.54	0/2994
All	All	0.46	0/26594	0.58	1/35930 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	118	ARG	NE-CZ-NH2	-7.66	116.47	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2167	0	2167	40	0
1	B	2158	0	2154	63	0
1	C	2158	0	2154	51	4
1	D	2167	0	2167	52	0
1	E	2158	0	2154	46	1
1	F	2158	0	2154	75	0
1	G	2154	0	2151	69	0
1	H	2154	0	2151	75	0
1	I	2154	0	2151	66	0
1	J	2154	0	2151	55	0
1	K	2158	0	2154	67	0
1	L	2158	0	2154	77	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
2	G	53	0	31	0	0
2	H	53	0	31	0	0
2	I	53	0	31	0	0
2	J	53	0	31	0	0
2	K	53	0	31	0	0
2	L	53	0	31	0	0
3	A	23	10	0	0	0
3	B	23	10	0	0	0
3	D	23	0	0	0	0
3	E	23	10	0	0	3
3	H	23	10	0	0	0
3	I	23	10	0	0	0
3	J	23	10	0	0	0
3	L	23	10	0	0	0
4	A	5	0	0	1	0
4	D	5	0	0	1	0
4	F	5	0	0	0	0
4	J	5	0	0	1	0
5	A	40	0	0	4	0
5	B	16	0	0	0	0
5	C	31	0	0	5	0
5	D	40	0	0	9	0
5	E	27	0	0	4	0
5	F	16	0	0	3	0
5	G	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	19	0	0	1	0
5	J	18	0	0	2	0
5	K	14	0	0	1	0
5	L	15	0	0	0	0
All	All	26987	70	26234	672	4

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 13.

All (672) 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:K:244:ASP:HA	1:K:247:LYS:HD3	1.32	1.11
1:J:244:ASP:HA	1:J:247:LYS:HD3	1.38	1.01
1:F:22:LYS:HZ1	1:F:38:GLU:HB3	1.26	0.99
1:K:49:ILE:HD11	1:L:48:PRO:HG3	1.45	0.98
1:A:49:ILE:HD11	1:D:48:PRO:HG3	1.41	0.97
1:K:48:PRO:HG3	1:L:49:ILE:HD11	1.46	0.95
1:K:50:ILE:HG22	1:K:118:ARG:HG2	1.47	0.95
1:A:238:MET:HE1	1:A:259:LEU:HD21	1.51	0.93
1:H:4:ARG:NH1	1:H:35:GLU:OE2	2.02	0.91
1:B:4:ARG:NH1	1:B:35:GLU:OE2	2.04	0.91
1:G:49:ILE:HD11	1:H:48:PRO:HG3	1.53	0.90
1:E:64:ASN:HB2	5:E:2403:HOH:O	1.72	0.90
1:B:244:ASP:HA	1:B:247:LYS:HD3	1.54	0.87
1:B:230:LEU:HD21	1:F:160:ILE:HD12	1.57	0.86
1:H:50:ILE:HG22	1:H:118:ARG:HG2	1.55	0.86
1:A:64:ASN:HB2	5:A:2433:HOH:O	1.76	0.85
1:D:76:LYS:HE3	1:D:123:GLU:HG3	1.59	0.85
1:F:22:LYS:NZ	1:F:38:GLU:HB3	1.93	0.84
1:K:60:LYS:O	1:K:62:PRO:HD3	1.77	0.84
1:H:89:LYS:NZ	1:H:92:GLU:OE1	2.09	0.83
1:I:238:MET:HE3	1:I:243:GLN:HG2	1.61	0.83
1:D:64:ASN:HB2	5:D:407:HOH:O	1.76	0.82
1:L:4:ARG:NH1	1:L:35:GLU:OE2	2.13	0.82
1:L:132:TYR:O	1:L:180:GLY:HA2	1.79	0.82
1:I:48:PRO:HG3	1:J:49:ILE:HD11	1.61	0.81
1:E:201:ILE:O	1:E:205:GLU:HG2	1.80	0.81
1:J:4:ARG:NH1	1:J:35:GLU:OE2	2.14	0.81
1:I:132:TYR:O	1:I:180:GLY:HA2	1.81	0.81
1:H:89:LYS:HE3	1:H:89:LYS:HA	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:LEU:HD22	1:F:22:LYS:HD2	1.62	0.80
1:G:4:ARG:HD2	1:G:93:ALA:O	1.81	0.79
1:J:76:LYS:HE3	1:J:123:GLU:HG3	1.63	0.79
1:J:189:THR:HG23	5:J:413:HOH:O	1.80	0.79
1:K:54:ASP:OD1	1:K:118:ARG:NH1	2.16	0.79
1:J:50:ILE:HG22	1:J:118:ARG:HG2	1.65	0.79
1:J:138:ARG:HA	1:J:180:GLY:O	1.82	0.79
1:J:141:LYS:NZ	1:J:215:TRP:O	2.16	0.79
1:C:201:ILE:O	1:C:205:GLU:HG2	1.83	0.79
1:B:48:PRO:HG3	1:F:49:ILE:HD11	1.63	0.78
1:I:198:ASP:O	1:I:202:GLN:HG2	1.83	0.78
1:I:201:ILE:O	1:I:205:GLU:HG2	1.84	0.78
1:F:89:LYS:NZ	1:F:92:GLU:OE1	2.17	0.78
1:G:260:GLY:O	1:H:262:SER:OG	2.02	0.77
1:E:32:LYS:HE3	1:E:212:GLU:HB3	1.66	0.77
1:G:230:LEU:CD2	1:H:160:ILE:HD12	2.16	0.76
1:K:189:THR:HG23	5:K:2409:HOH:O	1.84	0.76
1:L:141:LYS:NZ	1:L:215:TRP:O	2.17	0.76
1:D:4:ARG:NH1	1:D:35:GLU:OE2	2.19	0.76
1:G:138:ARG:HA	1:G:180:GLY:O	1.85	0.76
1:G:50:ILE:HG22	1:G:118:ARG:HG2	1.66	0.75
1:B:50:ILE:CG2	1:B:118:ARG:HG2	2.16	0.75
1:H:201:ILE:O	1:H:205:GLU:HG2	1.87	0.75
1:B:58:LYS:NZ	1:B:62:PRO:HG3	2.02	0.75
1:C:30:LYS:HE2	1:C:36:VAL:CG2	2.17	0.74
1:K:9:LEU:HD22	1:K:22:LYS:HD3	1.69	0.74
1:G:204:LEU:O	1:G:208:LYS:HG3	1.88	0.74
1:K:138:ARG:HA	1:K:180:GLY:O	1.88	0.74
1:K:50:ILE:CG2	1:K:118:ARG:HG2	2.17	0.73
1:G:201:ILE:O	1:G:205:GLU:HG2	1.88	0.73
1:H:54:ASP:OD1	1:H:118:ARG:NH1	2.21	0.73
1:K:230:LEU:HD21	1:L:160:ILE:HD12	1.70	0.73
1:H:30:LYS:HE2	1:H:36:VAL:HG22	1.69	0.73
1:D:238:MET:HE1	1:D:259:LEU:HD21	1.71	0.73
1:E:50:ILE:HG22	1:E:118:ARG:HG2	1.70	0.73
1:I:50:ILE:HG22	1:I:118:ARG:HG2	1.69	0.73
1:B:49:ILE:HD11	1:F:48:PRO:HG3	1.70	0.72
1:K:201:ILE:O	1:K:205:GLU:HG2	1.88	0.72
1:A:201:ILE:O	1:A:205:GLU:HG2	1.89	0.72
1:F:186:PRO:HB2	1:F:188:LEU:HD21	1.69	0.72
1:L:89:LYS:HA	1:L:89:LYS:HE3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:54:ASP:OD1	1:I:118:ARG:NH1	2.22	0.72
1:I:58:LYS:HD2	1:L:43:ALA:O	1.89	0.71
1:B:54:ASP:OD1	1:B:118:ARG:NH1	2.22	0.71
1:C:185:GLU:HG3	5:C:2414:HOH:O	1.89	0.71
1:G:9:LEU:HD22	1:G:22:LYS:HD3	1.71	0.71
1:C:238:MET:HE3	1:C:243:GLN:HG2	1.73	0.71
1:A:56:THR:O	1:A:56:THR:HG22	1.91	0.71
1:G:22:LYS:NZ	1:G:38:GLU:OE1	2.23	0.71
1:D:189:THR:HG23	5:D:423:HOH:O	1.90	0.70
1:L:244:ASP:HA	1:L:247:LYS:HD3	1.72	0.70
1:B:160:ILE:HD12	1:F:230:LEU:HD21	1.72	0.70
1:E:73:LEU:HD11	1:E:77:GLU:OE2	1.91	0.70
1:F:54:ASP:OD1	1:F:118:ARG:NH1	2.25	0.70
1:E:138:ARG:HA	1:E:180:GLY:O	1.92	0.70
1:K:40:ASP:O	1:K:44:MET:HG3	1.92	0.70
1:A:189:THR:HG23	5:A:2427:HOH:O	1.92	0.70
1:C:149:GLY:O	1:C:191:SER:HA	1.91	0.70
1:J:54:ASP:OD1	1:J:118:ARG:NH1	2.21	0.69
1:F:138:ARG:HA	1:F:180:GLY:O	1.93	0.69
1:C:138:ARG:HA	1:C:180:GLY:O	1.93	0.68
1:K:130:ALA:HB1	1:K:134:LYS:O	1.93	0.68
1:B:58:LYS:HZ2	1:B:62:PRO:HG3	1.59	0.68
1:E:189:THR:HG22	5:E:2423:HOH:O	1.93	0.68
1:B:130:ALA:O	1:B:135:GLY:HA2	1.93	0.68
1:H:204:LEU:O	1:H:208:LYS:HG3	1.94	0.68
1:C:89:LYS:NZ	1:C:92:GLU:OE1	2.26	0.68
1:I:244:ASP:HA	1:I:247:LYS:HD3	1.76	0.68
1:L:17:PHE:CE1	1:L:200:ARG:HG2	2.29	0.67
1:E:238:MET:HE3	1:E:243:GLN:HG2	1.76	0.67
1:B:138:ARG:HA	1:B:180:GLY:O	1.94	0.67
1:B:50:ILE:HG22	1:B:118:ARG:HG2	1.75	0.67
1:C:131:MET:HA	5:C:2401:HOH:O	1.93	0.67
1:L:113:LYS:O	1:L:117:GLU:HG3	1.94	0.67
1:C:30:LYS:HE2	1:C:36:VAL:HG21	1.77	0.67
1:G:141:LYS:NZ	1:G:215:TRP:O	2.27	0.67
1:K:132:TYR:O	1:K:180:GLY:HA2	1.93	0.67
1:B:22:LYS:NZ	1:B:23:GLU:OE2	2.26	0.67
1:K:185:GLU:OE2	1:K:271:ALA:N	2.21	0.67
1:H:128:TYR:CE1	1:H:236:PHE:HZ	2.13	0.67
1:F:204:LEU:O	1:F:208:LYS:HG3	1.93	0.67
1:B:68:PRO:O	1:B:72:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:LYS:O	1:E:117:GLU:HG3	1.95	0.66
1:L:201:ILE:O	1:L:205:GLU:HG2	1.95	0.66
1:C:50:ILE:HG22	1:C:118:ARG:HG2	1.77	0.66
1:E:211:LEU:HD23	1:E:214:ILE:HD13	1.77	0.66
1:K:218:THR:HG22	1:K:271:ALA:HB1	1.77	0.66
1:D:238:MET:CE	1:D:259:LEU:HD21	2.26	0.66
1:F:186:PRO:HB2	1:F:188:LEU:CD2	2.27	0.65
1:L:132:TYR:HA	1:L:177:HIS:O	1.96	0.65
1:B:160:ILE:HD12	1:F:230:LEU:CD2	2.27	0.65
1:C:189:THR:HG23	5:C:2409:HOH:O	1.96	0.65
1:H:130:ALA:O	1:H:135:GLY:HA2	1.97	0.65
1:C:36:VAL:HB	5:C:2424:HOH:O	1.96	0.65
1:D:238:MET:HE1	1:D:259:LEU:CD2	2.27	0.65
1:E:37:VAL:HG11	1:E:90:LYS:HG2	1.79	0.65
1:B:113:LYS:NZ	1:F:108:VAL:O	2.30	0.65
1:H:50:ILE:CG2	1:H:118:ARG:HG2	2.27	0.65
1:B:132:TYR:O	1:B:180:GLY:HA2	1.97	0.64
1:H:89:LYS:HA	1:H:89:LYS:CE	2.23	0.64
1:B:94:ALA:O	1:B:140:LYS:NZ	2.30	0.64
1:J:197:ALA:O	1:J:201:ILE:HG13	1.96	0.64
1:J:201:ILE:O	1:J:205:GLU:HG2	1.96	0.64
1:I:160:ILE:CD1	1:J:230:LEU:HD21	2.28	0.64
1:F:4:ARG:NH1	1:F:35:GLU:OE2	2.31	0.64
1:F:201:ILE:O	1:F:205:GLU:HG3	1.98	0.64
1:H:128:TYR:CE1	1:H:236:PHE:CZ	2.85	0.64
1:I:204:LEU:O	1:I:208:LYS:HG3	1.98	0.64
1:A:14:ARG:HG3	1:A:19:TYR:CZ	2.33	0.64
1:C:204:LEU:O	1:C:208:LYS:HG3	1.98	0.64
1:F:89:LYS:HE3	1:F:89:LYS:HA	1.80	0.64
1:J:200:ARG:NH2	4:J:303:SO4:O2	2.30	0.63
1:D:169:TRP:CZ2	1:D:256:GLY:HA3	2.33	0.63
1:F:22:LYS:NZ	1:F:38:GLU:OE1	2.30	0.63
1:H:246:GLU:O	1:H:261:LYS:NZ	2.30	0.63
1:F:73:LEU:HD11	1:F:77:GLU:OE2	1.99	0.63
1:I:50:ILE:HB	1:I:67:TYR:CE2	2.34	0.63
1:L:4:ARG:HD2	1:L:93:ALA:O	1.98	0.63
1:F:50:ILE:HG22	1:F:118:ARG:HG2	1.81	0.63
1:J:81:SER:OG	1:J:83:ASP:OD1	2.16	0.63
1:L:59:LEU:HD12	1:L:62:PRO:HB3	1.80	0.62
1:A:22:LYS:HE2	1:A:23:GLU:OE2	1.99	0.62
1:F:22:LYS:HZ1	1:F:38:GLU:CB	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91:LEU:HD11	1:K:120:PHE:HE1	1.63	0.62
1:B:238:MET:O	1:B:243:GLN:NE2	2.31	0.62
1:G:48:PRO:HG3	1:H:49:ILE:HD11	1.81	0.62
1:A:48:PRO:HG3	1:D:49:ILE:HD11	1.81	0.62
1:F:9:LEU:HD22	1:F:22:LYS:CD	2.29	0.62
1:F:89:LYS:HA	1:F:89:LYS:CE	2.30	0.62
1:L:133:ASP:OD1	1:L:225:SER:OG	2.16	0.61
1:G:50:ILE:CG2	1:G:118:ARG:HG2	2.31	0.61
1:I:30:LYS:HE2	1:I:36:VAL:CG2	2.30	0.61
1:L:55:ILE:HD12	1:L:55:ILE:H	1.66	0.61
1:J:60:LYS:O	1:J:60:LYS:HD3	2.01	0.61
1:A:202:GLN:OE1	1:A:202:GLN:HA	2.01	0.61
1:B:246:GLU:O	1:B:261:LYS:NZ	2.33	0.61
1:C:169:TRP:HB3	1:C:170:PRO:HD3	1.82	0.61
1:E:199:ALA:O	1:E:203:ILE:HG13	2.01	0.61
1:K:132:TYR:HA	1:K:177:HIS:O	2.00	0.61
1:D:132:TYR:O	1:D:180:GLY:HA2	2.01	0.61
1:E:189:THR:HG23	5:E:2419:HOH:O	1.99	0.61
1:J:50:ILE:CG2	1:J:118:ARG:HG2	2.30	0.61
1:L:73:LEU:HD11	1:L:77:GLU:OE2	2.00	0.61
1:L:55:ILE:HD12	1:L:55:ILE:N	2.17	0.60
1:C:4:ARG:HD2	1:C:93:ALA:O	2.01	0.60
1:K:200:ARG:HA	1:K:203:ILE:HD12	1.83	0.60
1:L:50:ILE:HG22	1:L:118:ARG:HG2	1.84	0.60
1:A:195:THR:CG2	1:A:199:ALA:HB3	2.32	0.60
1:B:158:GLN:HG2	1:F:243:GLN:OE1	2.01	0.60
1:B:50:ILE:HG23	1:B:118:ARG:HG2	1.83	0.60
1:E:238:MET:CE	1:E:243:GLN:HG2	2.32	0.60
1:F:76:LYS:HE2	1:F:123:GLU:HG3	1.83	0.60
1:I:224:PRO:HD2	1:I:227:LEU:HD11	1.84	0.59
1:K:145:SER:HA	1:K:187:GLN:HB3	1.84	0.59
1:G:49:ILE:HD11	1:H:48:PRO:CG	2.30	0.59
1:C:60:LYS:HD3	1:C:60:LYS:O	2.03	0.59
1:E:144:LEU:HD21	1:E:176:LEU:HD11	1.83	0.59
1:H:22:LYS:NZ	1:H:38:GLU:OE1	2.31	0.59
1:H:127:THR:O	1:H:131:MET:HE3	2.03	0.59
1:H:128:TYR:HH	1:H:236:PHE:HZ	1.50	0.59
1:L:7:ILE:HG21	1:L:22:LYS:HG2	1.82	0.59
1:G:89:LYS:HA	1:G:89:LYS:CE	2.33	0.59
1:I:88:GLN:HG2	1:I:124:PHE:CE2	2.38	0.59
1:I:30:LYS:HE2	1:I:36:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:LEU:HD13	5:E:2424:HOH:O	2.02	0.58
1:F:75:TYR:CZ	1:F:124:PHE:HB2	2.38	0.58
1:K:244:ASP:HA	1:K:247:LYS:CD	2.21	0.58
1:L:89:LYS:NZ	1:L:92:GLU:OE1	2.34	0.58
1:E:50:ILE:CG2	1:E:118:ARG:HG2	2.33	0.58
1:J:132:TYR:O	1:J:180:GLY:HA2	2.03	0.58
1:K:197:ALA:O	1:K:201:ILE:HG13	2.02	0.58
1:C:25:ALA:HA	1:C:211:LEU:CD1	2.34	0.58
1:D:138:ARG:HA	1:D:180:GLY:O	2.02	0.58
1:B:4:ARG:HD2	1:B:93:ALA:O	2.03	0.58
1:G:76:LYS:HE3	1:G:123:GLU:HG3	1.84	0.58
1:I:158:GLN:HG2	1:J:243:GLN:OE1	2.04	0.58
1:D:106:PHE:HD1	1:D:167:ILE:HD13	1.68	0.58
1:G:130:ALA:O	1:G:135:GLY:HA2	2.03	0.58
1:C:238:MET:HE3	1:C:243:GLN:CG	2.33	0.58
1:K:244:ASP:CA	1:K:247:LYS:HD3	2.20	0.58
1:F:14:ARG:HG3	1:F:19:TYR:CE1	2.39	0.57
1:F:169:TRP:CZ2	1:F:256:GLY:HA3	2.39	0.57
1:A:178:PHE:HE1	1:D:161:HIS:HE1	1.53	0.57
1:A:238:MET:CE	1:A:259:LEU:HD21	2.30	0.57
1:F:55:ILE:N	1:F:55:ILE:HD12	2.19	0.57
1:G:132:TYR:HA	1:G:177:HIS:O	2.04	0.57
1:B:238:MET:CE	1:B:243:GLN:HG2	2.34	0.57
1:H:91:LEU:HD11	1:H:120:PHE:HE1	1.69	0.57
1:J:122:GLY:O	1:J:123:GLU:HB2	2.03	0.57
1:K:238:MET:HG3	1:L:158:GLN:HB3	1.87	0.57
1:L:169:TRP:HB3	1:L:170:PRO:HD3	1.86	0.57
1:E:198:ASP:HA	1:E:201:ILE:HD12	1.85	0.57
1:I:49:ILE:HD11	1:J:48:PRO:HG3	1.86	0.57
1:L:29:LEU:O	1:L:34:TRP:HB2	2.03	0.57
1:F:22:LYS:HD3	5:F:2403:HOH:O	2.05	0.57
1:C:53:LYS:HD3	1:D:14:ARG:HH12	1.70	0.57
1:F:130:ALA:O	1:F:135:GLY:HA2	2.05	0.57
1:H:128:TYR:HE1	1:H:236:PHE:CZ	2.21	0.56
1:J:68:PRO:O	1:J:72:VAL:HG23	2.05	0.56
1:K:173:SER:HB2	1:K:222:PHE:CE2	2.40	0.56
1:A:169:TRP:HB3	1:A:170:PRO:HD3	1.87	0.56
1:F:50:ILE:CG2	1:F:118:ARG:HG2	2.35	0.56
1:A:197:ALA:O	1:A:201:ILE:HG13	2.06	0.56
1:L:138:ARG:HA	1:L:180:GLY:O	2.05	0.56
1:E:55:ILE:HG12	1:E:74:ALA:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:ARG:HD2	1:F:93:ALA:O	2.06	0.56
1:G:132:TYR:CD1	1:G:178:PHE:HA	2.41	0.56
1:K:135:GLY:O	1:K:138:ARG:NH1	2.34	0.56
1:L:54:ASP:OD1	1:L:118:ARG:NH1	2.35	0.56
1:L:210:ARG:O	1:L:210:ARG:HG2	2.05	0.56
1:A:200:ARG:NH2	4:A:2303:SO4:O1	2.39	0.56
1:I:138:ARG:HA	1:I:180:GLY:O	2.06	0.56
1:G:238:MET:HB3	1:G:243:GLN:CG	2.35	0.56
1:L:149:GLY:O	1:L:191:SER:HA	2.04	0.56
1:D:28:ALA:HB2	1:D:208:LYS:HG2	1.88	0.56
1:L:238:MET:CE	1:L:259:LEU:HD21	2.36	0.56
1:G:25:ALA:HB2	1:G:207:TRP:HE1	1.71	0.55
1:D:4:ARG:HD2	1:D:93:ALA:O	2.06	0.55
1:G:89:LYS:HA	1:G:89:LYS:HE3	1.88	0.55
1:D:249:LYS:HD3	5:D:437:HOH:O	2.06	0.55
1:I:69:ALA:HB2	5:I:2409:HOH:O	2.06	0.55
1:K:30:LYS:HG3	1:K:36:VAL:CG1	2.37	0.55
1:B:201:ILE:O	1:B:205:GLU:HG2	2.07	0.55
1:A:138:ARG:HA	1:A:180:GLY:O	2.07	0.55
1:H:128:TYR:CZ	1:H:236:PHE:HZ	2.24	0.55
1:B:147:THR:HG22	1:B:189:THR:OG1	2.07	0.55
1:H:185:GLU:OE2	1:H:270:LYS:HA	2.06	0.55
1:I:160:ILE:HD13	1:J:230:LEU:HD21	1.87	0.55
1:G:246:GLU:HA	1:G:249:LYS:HG3	1.88	0.54
1:J:132:TYR:CD1	1:J:178:PHE:HA	2.42	0.54
1:K:30:LYS:HG3	1:K:36:VAL:HG13	1.89	0.54
1:H:72:VAL:CG2	1:H:122:GLY:HA3	2.37	0.54
1:A:204:LEU:O	1:A:208:LYS:HG3	2.07	0.54
1:K:238:MET:CE	1:K:242:VAL:HG12	2.36	0.54
1:D:201:ILE:O	1:D:205:GLU:HG2	2.07	0.54
1:F:29:LEU:CD1	1:F:211:LEU:HB3	2.37	0.54
1:H:198:ASP:O	1:H:202:GLN:HG2	2.07	0.54
1:C:241:GLU:OE1	1:C:241:GLU:N	2.25	0.54
1:J:113:LYS:O	1:J:117:GLU:HG3	2.08	0.54
1:A:229:ASP:OD1	1:A:239:LYS:HG2	2.07	0.53
1:B:263:ILE:HD11	1:F:263:ILE:HD11	1.91	0.53
1:G:11:HIS:CE1	1:G:16:SER:HB3	2.43	0.53
1:J:261:LYS:HE2	5:J:418:HOH:O	2.08	0.53
1:C:4:ARG:NH1	1:C:35:GLU:OE2	2.40	0.53
1:D:248:ASN:HB3	5:D:410:HOH:O	2.06	0.53
1:F:227:LEU:HB3	1:F:242:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:ASP:OD1	1:E:239:LYS:HG2	2.09	0.53
1:J:38:GLU:O	1:J:90:LYS:NZ	2.33	0.53
1:E:130:ALA:HB1	1:E:134:LYS:O	2.08	0.53
1:L:122:GLY:O	1:L:123:GLU:HB2	2.09	0.53
1:J:120:PHE:HA	1:J:125:ALA:HB2	1.90	0.53
1:L:36:VAL:HG23	1:L:36:VAL:O	2.08	0.53
1:F:132:TYR:O	1:F:180:GLY:HA2	2.08	0.53
1:H:37:VAL:HG12	1:H:38:GLU:N	2.24	0.53
1:H:144:LEU:HD21	1:H:176:LEU:HD11	1.91	0.53
1:D:261:LYS:HE2	5:D:438:HOH:O	2.09	0.53
1:H:25:ALA:HB2	1:H:207:TRP:HE1	1.74	0.53
1:G:128:TYR:CE1	1:G:232:PHE:CE2	2.97	0.52
1:K:118:ARG:O	1:K:121:ILE:HD11	2.08	0.52
1:I:160:ILE:HD13	1:J:230:LEU:CD2	2.39	0.52
1:B:81:SER:OG	1:B:83:ASP:OD1	2.17	0.52
1:H:76:LYS:HE3	1:H:123:GLU:HG3	1.92	0.52
1:L:176:LEU:O	1:L:181:PHE:HB2	2.09	0.52
1:D:141:LYS:HD3	1:D:184:LEU:HD21	1.92	0.52
1:G:155:TYR:HB3	1:G:164:MET:HB2	1.92	0.52
1:H:128:TYR:OH	1:H:236:PHE:HZ	1.93	0.52
1:K:4:ARG:HD3	1:K:35:GLU:OE2	2.10	0.52
1:K:75:TYR:CZ	1:K:124:PHE:HB2	2.44	0.52
1:D:91:LEU:HD11	1:D:120:PHE:HE1	1.73	0.52
1:I:149:GLY:O	1:I:191:SER:HA	2.09	0.52
1:B:127:THR:OG1	1:B:130:ALA:HB3	2.10	0.52
1:C:225:SER:HB2	1:C:230:LEU:HD11	1.91	0.51
1:D:58:LYS:NZ	1:D:62:PRO:HG3	2.26	0.51
1:E:22:LYS:HE3	1:E:38:GLU:OE1	2.09	0.51
1:F:167:ILE:O	1:F:170:PRO:HD2	2.10	0.51
1:I:160:ILE:HD12	1:J:230:LEU:HD21	1.92	0.51
1:I:58:LYS:HG3	1:I:59:LEU:N	2.25	0.51
1:F:241:GLU:H	1:F:241:GLU:CD	2.12	0.51
1:I:239:LYS:O	1:I:243:GLN:HG3	2.10	0.51
1:E:204:LEU:O	1:E:208:LYS:HG3	2.10	0.51
1:J:43:ALA:HB1	1:K:82:PRO:HD2	1.93	0.51
1:K:128:TYR:CE2	1:K:236:PHE:HZ	2.28	0.51
1:L:229:ASP:O	1:L:236:PHE:HA	2.10	0.51
1:L:238:MET:HE1	1:L:259:LEU:HD21	1.91	0.51
1:G:239:LYS:O	1:G:243:GLN:HG3	2.11	0.51
5:A:2420:HOH:O	1:D:52:ARG:HD3	2.10	0.51
1:I:91:LEU:HD11	1:I:120:PHE:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LEU:O	1:C:77:GLU:HG3	2.10	0.51
1:K:52:ARG:HA	1:K:65:PHE:CZ	2.46	0.51
1:L:128:TYR:CZ	1:L:236:PHE:HZ	2.29	0.51
1:B:250:LYS:O	1:B:261:LYS:HB3	2.10	0.50
1:C:56:THR:HA	1:D:14:ARG:HH21	1.75	0.50
1:D:239:LYS:NZ	4:D:303:SO4:O2	2.44	0.50
1:J:172:GLN:HB3	1:J:183:VAL:HG11	1.92	0.50
1:F:189:THR:HG23	5:F:2406:HOH:O	2.11	0.50
1:K:238:MET:HE1	1:K:242:VAL:HG12	1.93	0.50
1:L:49:ILE:O	1:L:118:ARG:HD3	2.12	0.50
1:C:130:ALA:HB1	1:C:134:LYS:O	2.11	0.50
1:G:109:PRO:HA	1:H:117:GLU:OE2	2.12	0.50
1:K:55:ILE:N	1:K:55:ILE:HD12	2.27	0.50
1:D:50:ILE:CG2	1:D:118:ARG:HG2	2.42	0.50
1:L:94:ALA:O	1:L:140:LYS:NZ	2.43	0.50
1:I:132:TYR:HA	1:I:177:HIS:O	2.12	0.50
1:A:169:TRP:CZ2	1:A:256:GLY:HA3	2.46	0.50
1:K:211:LEU:HA	1:K:214:ILE:HB	1.93	0.50
1:L:128:TYR:CE1	1:L:236:PHE:CZ	3.00	0.50
1:H:48:PRO:C	1:H:49:ILE:HD13	2.32	0.50
1:K:29:LEU:CD1	1:K:211:LEU:HB3	2.41	0.50
1:L:165:ASN:OD1	1:L:266:ASP:HA	2.11	0.50
1:E:132:TYR:O	1:E:180:GLY:HA2	2.12	0.50
1:G:68:PRO:O	1:G:72:VAL:HG23	2.12	0.50
1:H:59:LEU:HD12	1:H:62:PRO:HB3	1.94	0.50
1:I:13:GLU:OE1	1:J:52:ARG:NH1	2.45	0.50
1:I:165:ASN:HD21	1:I:266:ASP:HA	1.76	0.50
1:K:155:TYR:HB3	1:K:164:MET:HB2	1.94	0.50
1:B:60:LYS:O	1:B:60:LYS:HD3	2.11	0.49
1:K:128:TYR:HE2	1:K:236:PHE:HZ	1.60	0.49
1:C:229:ASP:O	1:C:236:PHE:HA	2.11	0.49
1:F:32:LYS:HE3	1:F:212:GLU:HB3	1.94	0.49
1:H:138:ARG:HA	1:H:180:GLY:O	2.13	0.49
1:H:173:SER:HB2	1:H:222:PHE:CE1	2.46	0.49
1:L:14:ARG:HG2	1:L:19:TYR:CZ	2.47	0.49
1:B:105:TRP:HB3	1:F:175:ILE:HG12	1.94	0.49
1:B:238:MET:HE2	1:B:243:GLN:HG2	1.94	0.49
1:I:4:ARG:HD2	1:I:93:ALA:O	2.12	0.49
1:A:132:TYR:O	1:A:180:GLY:HA2	2.12	0.49
1:A:229:ASP:O	1:A:236:PHE:HA	2.13	0.49
1:B:132:TYR:OH	1:F:161:HIS:ND1	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:HG22	1:A:199:ALA:HB3	1.95	0.49
1:A:230:LEU:HD21	1:D:160:ILE:HD12	1.95	0.49
1:F:152:GLY:HA2	1:F:190:TYR:CD1	2.47	0.49
1:G:3:ARG:O	1:G:3:ARG:HG2	2.13	0.49
1:H:4:ARG:HD2	1:H:93:ALA:O	2.13	0.49
1:A:106:PHE:CD2	1:D:174:GLY:HA3	2.48	0.49
1:I:122:GLY:O	1:I:123:GLU:HB2	2.12	0.49
1:A:132:TYR:HA	1:A:177:HIS:O	2.12	0.48
1:E:132:TYR:CD1	1:E:178:PHE:HA	2.48	0.48
1:G:37:VAL:HG11	1:G:90:LYS:HG2	1.95	0.48
1:G:48:PRO:O	1:G:114:GLY:HA3	2.12	0.48
1:J:132:TYR:HA	1:J:177:HIS:O	2.12	0.48
1:G:128:TYR:CE1	1:G:236:PHE:HZ	2.32	0.48
1:J:31:LYS:O	1:J:31:LYS:HG2	2.13	0.48
1:B:58:LYS:HZ1	1:B:62:PRO:HG3	1.76	0.48
1:D:132:TYR:HA	1:D:177:HIS:O	2.12	0.48
1:K:36:VAL:O	1:K:36:VAL:CG2	2.61	0.48
1:B:85:VAL:O	1:B:89:LYS:HG2	2.13	0.48
1:C:25:ALA:HA	1:C:211:LEU:HD12	1.95	0.48
1:I:130:ALA:O	1:I:135:GLY:HA2	2.13	0.48
1:B:95:ASP:HB3	1:B:215:TRP:CH2	2.48	0.48
1:E:244:ASP:HA	1:E:247:LYS:HD3	1.94	0.48
1:I:14:ARG:HG3	1:I:19:TYR:CZ	2.48	0.48
1:I:40:ASP:O	1:I:44:MET:HG3	2.14	0.48
1:G:132:TYR:O	1:G:180:GLY:HA2	2.13	0.48
1:G:174:GLY:O	1:H:106:PHE:CE2	2.66	0.48
1:I:224:PRO:O	1:I:227:LEU:HG	2.14	0.48
1:L:50:ILE:CG2	1:L:118:ARG:HG2	2.43	0.48
1:E:54:ASP:OD1	1:E:118:ARG:NH1	2.31	0.48
1:B:29:LEU:O	1:B:34:TRP:HB2	2.14	0.48
1:C:141:LYS:HD2	1:C:215:TRP:CE3	2.49	0.48
1:D:226:SER:O	1:D:239:LYS:NZ	2.46	0.48
1:G:54:ASP:OD1	1:G:118:ARG:NH1	2.35	0.48
1:I:50:ILE:CG2	1:I:118:ARG:HG2	2.42	0.48
1:K:37:VAL:HG11	1:K:90:LYS:HG2	1.96	0.48
1:L:132:TYR:CD1	1:L:178:PHE:HA	2.48	0.48
1:G:48:PRO:CG	1:H:49:ILE:HD11	2.44	0.48
1:G:176:LEU:O	1:G:181:PHE:HB2	2.14	0.48
1:K:46:PHE:O	1:K:48:PRO:HD3	2.14	0.48
1:C:36:VAL:HG23	1:C:36:VAL:O	2.14	0.48
1:D:50:ILE:HG23	1:D:118:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:TYR:CE1	1:H:22:LYS:HE2	2.48	0.48
1:I:165:ASN:ND2	1:I:266:ASP:HA	2.29	0.48
1:L:155:TYR:HB3	1:L:164:MET:HB2	1.95	0.48
1:G:14:ARG:HG2	1:G:19:TYR:CZ	2.49	0.47
1:J:155:TYR:HB3	1:J:164:MET:HB2	1.96	0.47
1:L:75:TYR:CZ	1:L:124:PHE:HB2	2.48	0.47
1:L:76:LYS:HE3	1:L:123:GLU:HG3	1.96	0.47
1:B:155:TYR:HB3	1:B:164:MET:HB2	1.96	0.47
1:D:185:GLU:HG3	5:D:419:HOH:O	2.13	0.47
1:F:106:PHE:HD2	1:F:167:ILE:HD13	1.78	0.47
1:G:89:LYS:HZ2	1:G:92:GLU:HB2	1.79	0.47
1:L:32:LYS:HE3	1:L:212:GLU:HB3	1.96	0.47
1:B:230:LEU:CD2	1:F:160:ILE:HD12	2.36	0.47
1:I:141:LYS:NZ	1:I:215:TRP:O	2.48	0.47
1:B:132:TYR:CD1	1:B:178:PHE:HA	2.50	0.47
1:J:204:LEU:O	1:J:208:LYS:HG3	2.14	0.47
1:G:108:VAL:O	1:H:113:LYS:NZ	2.48	0.47
1:I:14:ARG:HG3	1:I:19:TYR:CE2	2.48	0.47
1:J:246:GLU:HA	1:J:249:LYS:HG3	1.95	0.47
1:L:143:VAL:HG23	1:L:185:GLU:O	2.14	0.47
1:B:149:GLY:O	1:B:191:SER:HA	2.15	0.47
1:B:232:PHE:HA	1:B:236:PHE:CE1	2.49	0.47
1:C:130:ALA:O	1:C:135:GLY:HA2	2.14	0.47
1:G:160:ILE:HG13	1:G:160:ILE:O	2.14	0.47
1:I:132:TYR:CE2	1:J:160:ILE:HD13	2.50	0.47
1:F:29:LEU:O	1:F:34:TRP:HB2	2.15	0.47
1:D:67:TYR:N	1:D:68:PRO:CD	2.78	0.47
1:D:155:TYR:HB3	1:D:164:MET:HB2	1.97	0.47
1:E:130:ALA:O	1:E:135:GLY:HA2	2.16	0.47
1:F:6:LEU:HA	1:F:37:VAL:O	2.15	0.47
1:L:106:PHE:HD1	1:L:167:ILE:HD13	1.80	0.47
1:L:169:TRP:CZ2	1:L:256:GLY:HA3	2.50	0.47
1:E:6:LEU:HA	1:E:37:VAL:O	2.15	0.46
1:H:173:SER:HB2	1:H:222:PHE:HE1	1.79	0.46
1:L:89:LYS:HD2	1:L:89:LYS:N	2.29	0.46
1:G:53:LYS:HD3	1:G:53:LYS:HA	1.35	0.46
1:K:7:ILE:HG21	1:K:22:LYS:HG3	1.97	0.46
1:K:94:ALA:O	1:K:140:LYS:NZ	2.44	0.46
1:D:103:LEU:HB3	1:D:148:THR:HG22	1.97	0.46
1:F:147:THR:HG22	1:F:189:THR:OG1	2.16	0.46
1:B:173:SER:HB2	1:B:222:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:118:ARG:O	1:J:121:ILE:HD11	2.15	0.46
1:K:49:ILE:HD11	1:L:48:PRO:CG	2.31	0.46
1:B:169:TRP:CZ2	1:B:256:GLY:HA3	2.50	0.46
1:B:197:ALA:HA	1:B:200:ARG:CZ	2.45	0.46
1:H:9:LEU:HD22	1:H:22:LYS:HD3	1.97	0.46
1:K:240:LYS:HB3	1:K:240:LYS:HE3	1.71	0.46
1:E:155:TYR:HB3	1:E:164:MET:HB2	1.97	0.46
1:G:29:LEU:O	1:G:34:TRP:HB2	2.15	0.46
1:G:174:GLY:O	1:H:106:PHE:HE2	1.99	0.46
1:I:11:HIS:CD2	1:I:18:ASN:HB2	2.51	0.46
1:I:132:TYR:HE2	1:J:160:ILE:HD13	1.81	0.46
1:K:247:LYS:HE2	1:K:247:LYS:HB2	1.50	0.46
1:B:239:LYS:O	1:B:243:GLN:HG3	2.16	0.46
1:I:9:LEU:HD23	1:I:40:ASP:OD2	2.15	0.46
1:A:14:ARG:HG3	1:A:19:TYR:CE2	2.51	0.46
1:G:169:TRP:CZ2	1:G:256:GLY:HA3	2.51	0.46
1:J:76:LYS:CE	1:J:123:GLU:HG3	2.41	0.46
1:A:141:LYS:HE3	1:A:215:TRP:CZ2	2.51	0.46
1:F:197:ALA:HA	1:F:200:ARG:CZ	2.46	0.46
1:H:72:VAL:HG22	1:H:122:GLY:HA3	1.98	0.46
1:D:229:ASP:O	1:D:236:PHE:HA	2.16	0.46
1:G:130:ALA:HB1	1:G:134:LYS:O	2.16	0.46
1:H:30:LYS:HE2	1:H:36:VAL:CG2	2.43	0.46
1:H:91:LEU:HD23	1:H:91:LEU:HA	1.80	0.46
1:K:30:LYS:CG	1:K:36:VAL:HG13	2.46	0.46
1:L:128:TYR:OH	1:L:236:PHE:HZ	1.99	0.46
1:C:66:GLN:O	1:C:70:GLU:HG2	2.15	0.45
1:H:128:TYR:HA	1:H:131:MET:HE3	1.98	0.45
1:L:252:GLY:O	1:L:264:PRO:HG3	2.16	0.45
5:A:2435:HOH:O	1:D:232:PHE:HD1	1.99	0.45
1:C:144:LEU:HD21	1:C:176:LEU:HD11	1.97	0.45
1:E:58:LYS:HG3	1:E:59:LEU:N	2.31	0.45
1:E:153:SER:O	1:E:159:GLY:HA3	2.16	0.45
1:F:9:LEU:HB3	1:F:22:LYS:HE3	1.98	0.45
1:I:48:PRO:O	1:I:114:GLY:HA3	2.15	0.45
1:J:238:MET:HB3	1:J:243:GLN:HG3	1.97	0.45
1:E:89:LYS:NZ	1:E:92:GLU:OE1	2.49	0.45
1:G:14:ARG:HG2	1:G:19:TYR:CE1	2.51	0.45
1:K:49:ILE:CD1	1:L:48:PRO:HG3	2.32	0.45
1:E:28:ALA:HB2	1:E:208:LYS:HE3	1.98	0.45
1:E:54:ASP:OD1	1:E:118:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:HIS:HE1	1:H:178:PHE:HE2	1.65	0.45
1:J:4:ARG:HD2	1:J:93:ALA:O	2.17	0.45
1:G:148:THR:OG1	1:G:190:TYR:HA	2.16	0.45
1:H:239:LYS:O	1:H:243:GLN:HG3	2.16	0.45
1:A:106:PHE:HD1	1:A:167:ILE:HD13	1.82	0.45
1:B:105:TRP:HB2	1:F:113:LYS:HE3	1.99	0.45
1:F:176:LEU:O	1:F:181:PHE:HB2	2.17	0.45
1:J:238:MET:HE1	1:J:253:LEU:HD12	1.99	0.45
1:G:25:ALA:HB2	1:G:207:TRP:NE1	2.30	0.45
1:H:151:SER:OG	1:H:154:MET:HG3	2.17	0.45
1:F:106:PHE:HD2	1:F:167:ILE:CD1	2.30	0.45
1:G:132:TYR:OH	1:H:161:HIS:ND1	2.41	0.45
1:I:82:PRO:HB3	1:L:56:THR:HG22	1.98	0.45
1:B:41:LEU:HD21	1:B:115:TRP:CD1	2.52	0.45
1:B:238:MET:HE3	1:B:243:GLN:HG2	1.98	0.45
1:H:234:ALA:O	1:H:237:LEU:HG	2.17	0.45
1:F:9:LEU:CD2	1:F:22:LYS:HD2	2.41	0.44
1:I:113:LYS:NZ	1:J:104:GLN:O	2.44	0.44
1:E:106:PHE:HD1	1:E:167:ILE:HD13	1.82	0.44
1:J:55:ILE:HG12	1:J:74:ALA:HB2	1.99	0.44
1:J:169:TRP:CZ2	1:J:256:GLY:HA3	2.53	0.44
1:D:226:SER:HA	5:D:430:HOH:O	2.18	0.44
1:I:208:LYS:HE2	1:I:208:LYS:HB3	1.83	0.44
1:A:108:VAL:HB	1:A:112:LEU:HD23	2.00	0.44
1:E:67:TYR:N	1:E:68:PRO:CD	2.80	0.44
1:F:14:ARG:HG3	1:F:19:TYR:CZ	2.53	0.44
1:G:45:ASN:ND2	5:G:2401:HOH:O	2.50	0.44
1:H:22:LYS:HE3	1:H:23:GLU:HG2	1.99	0.44
1:E:106:PHE:HD1	1:E:167:ILE:CD1	2.30	0.44
1:F:101:PHE:CZ	1:F:108:VAL:HG12	2.53	0.44
1:L:75:TYR:CE1	1:L:124:PHE:HB2	2.53	0.44
1:F:133:ASP:OD2	1:F:224:PRO:HA	2.18	0.44
1:A:230:LEU:CD2	1:D:160:ILE:HD12	2.47	0.44
1:F:72:VAL:O	1:F:75:TYR:HB3	2.18	0.44
1:G:214:ILE:O	1:G:214:ILE:HG13	2.17	0.44
1:I:36:VAL:O	1:I:36:VAL:HG23	2.18	0.44
1:J:32:LYS:HE3	1:J:212:GLU:HG2	1.98	0.44
1:B:141:LYS:HG2	1:B:182:GLN:HB2	2.00	0.44
1:L:53:LYS:HD3	1:L:53:LYS:HA	1.48	0.44
1:C:122:GLY:O	1:C:123:GLU:HB2	2.18	0.44
1:D:227:LEU:HB3	1:D:242:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:LYS:HA	1:E:134:LYS:HD3	1.83	0.44
1:F:141:LYS:HG2	1:F:182:GLN:HB2	2.00	0.44
1:B:109:PRO:HA	1:F:117:GLU:OE2	2.17	0.43
1:C:88:GLN:HG2	1:C:124:PHE:CE2	2.53	0.43
1:H:72:VAL:HG22	1:H:122:GLY:CA	2.48	0.43
1:C:32:LYS:HE3	1:C:212:GLU:HB3	2.01	0.43
1:G:4:ARG:NH1	1:G:35:GLU:OE2	2.51	0.43
1:H:55:ILE:N	1:H:55:ILE:HD12	2.33	0.43
1:J:31:LYS:O	1:J:31:LYS:CG	2.67	0.43
1:E:214:ILE:HG23	1:E:215:TRP:N	2.33	0.43
1:H:80:LEU:O	1:H:81:SER:C	2.57	0.43
1:I:187:GLN:OE1	1:I:187:GLN:HA	2.18	0.43
1:L:141:LYS:HD2	1:L:215:TRP:CE3	2.54	0.43
1:A:14:ARG:HG3	1:A:19:TYR:CE1	2.54	0.43
1:D:241:GLU:CD	1:D:241:GLU:H	2.22	0.43
1:H:241:GLU:H	1:H:241:GLU:CD	2.20	0.43
1:A:243:GLN:OE1	1:D:158:GLN:HG2	2.17	0.43
1:C:14:ARG:HG2	1:C:19:TYR:CE2	2.53	0.43
1:C:132:TYR:HA	1:C:177:HIS:O	2.18	0.43
1:I:169:TRP:HB3	1:I:170:PRO:HD3	2.00	0.43
1:A:123:GLU:N	1:A:126:TYR:O	2.46	0.43
1:C:165:ASN:OD1	1:C:266:ASP:HA	2.19	0.43
1:H:132:TYR:O	1:H:180:GLY:HA2	2.19	0.43
1:H:238:MET:HB3	1:H:243:GLN:HG2	2.00	0.43
1:L:36:VAL:O	1:L:36:VAL:CG2	2.66	0.43
1:L:229:ASP:HB2	1:L:234:ALA:HB1	2.00	0.43
1:A:250:LYS:HD3	1:A:251:PHE:CE2	2.54	0.43
1:H:81:SER:OG	1:H:83:ASP:OD1	2.31	0.43
1:H:195:THR:CG2	1:H:199:ALA:HB3	2.49	0.43
1:I:148:THR:OG1	1:I:190:TYR:HA	2.19	0.43
1:I:155:TYR:HB3	1:I:164:MET:HB2	2.00	0.43
1:C:3:ARG:HA	1:C:3:ARG:HD3	1.64	0.43
1:D:54:ASP:OD1	1:D:118:ARG:NH1	2.40	0.43
1:F:22:LYS:HG2	5:F:2403:HOH:O	2.19	0.43
1:G:128:TYR:CE1	1:G:236:PHE:CZ	3.07	0.43
1:I:229:ASP:OD1	1:I:239:LYS:HG2	2.18	0.43
1:L:89:LYS:HA	1:L:89:LYS:CE	2.40	0.43
1:A:9:LEU:HD22	1:A:22:LYS:HD3	2.00	0.43
1:B:88:GLN:HG2	1:B:124:PHE:CE2	2.54	0.43
1:B:232:PHE:CD1	1:B:236:PHE:HE1	2.35	0.43
1:C:50:ILE:CG2	1:C:118:ARG:HG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:HIS:HB3	1:E:263:ILE:HG12	2.01	0.42
1:G:166:VAL:HG13	1:H:166:VAL:HG13	2.00	0.42
1:G:238:MET:HB3	1:G:243:GLN:HG3	2.01	0.42
1:A:173:SER:HB2	1:A:222:PHE:CE2	2.55	0.42
1:G:11:HIS:CE1	1:G:16:SER:CB	3.02	0.42
1:A:122:GLY:O	1:A:123:GLU:HB3	2.19	0.42
1:C:232:PHE:CD1	1:C:236:PHE:HE2	2.38	0.42
1:F:29:LEU:HD11	1:F:211:LEU:HB3	2.01	0.42
1:K:14:ARG:HD2	1:K:19:TYR:CZ	2.54	0.42
1:K:25:ALA:HA	1:K:211:LEU:CD1	2.50	0.42
1:K:128:TYR:CD1	1:K:128:TYR:C	2.92	0.42
1:I:204:LEU:HD23	1:I:204:LEU:HA	1.85	0.42
1:J:11:HIS:CE1	1:J:16:SER:HB3	2.54	0.42
1:K:173:SER:HB2	1:K:222:PHE:HE2	1.84	0.42
1:K:174:GLY:O	1:L:106:PHE:CE2	2.72	0.42
1:K:263:ILE:HD11	1:L:263:ILE:HD11	2.01	0.42
1:L:48:PRO:O	1:L:114:GLY:HA3	2.19	0.42
1:L:86:ALA:O	1:L:90:LYS:HG3	2.19	0.42
1:L:128:TYR:CE1	1:L:236:PHE:HZ	2.37	0.42
1:B:108:VAL:HB	1:B:112:LEU:HD23	2.02	0.42
1:D:169:TRP:HB3	1:D:170:PRO:HD3	2.01	0.42
1:H:59:LEU:HB2	1:H:62:PRO:HB3	2.01	0.42
1:H:195:THR:HG22	1:H:199:ALA:HB3	2.00	0.42
1:I:196:PRO:HD2	1:I:199:ALA:HB3	2.00	0.42
1:F:9:LEU:HB2	1:F:22:LYS:HD2	2.01	0.42
1:F:207:TRP:O	1:F:211:LEU:HG	2.18	0.42
1:I:173:SER:HA	1:I:177:HIS:HB3	2.01	0.42
1:B:7:ILE:HG21	1:B:22:LYS:HG2	2.02	0.42
1:F:68:PRO:O	1:F:72:VAL:HG23	2.20	0.42
1:H:91:LEU:CD1	1:H:120:PHE:HE1	2.33	0.42
1:A:151:SER:OG	1:A:154:MET:HG3	2.19	0.42
1:C:36:VAL:CB	5:C:2424:HOH:O	2.64	0.42
1:D:132:TYR:CD1	1:D:178:PHE:HA	2.54	0.42
1:E:5:ALA:O	1:E:36:VAL:HA	2.19	0.42
1:G:6:LEU:HA	1:G:37:VAL:O	2.19	0.42
1:I:56:THR:CG2	1:I:81:SER:HA	2.50	0.42
1:I:73:LEU:O	1:I:77:GLU:HG3	2.20	0.42
1:I:98:ILE:HG12	1:I:143:VAL:CG1	2.49	0.42
1:B:173:SER:HA	1:B:177:HIS:HB3	2.02	0.42
1:C:169:TRP:CZ2	1:C:256:GLY:HA3	2.55	0.42
1:I:229:ASP:O	1:I:236:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:THR:O	1:L:79:HIS:HB3	2.20	0.42
1:I:36:VAL:CG2	1:I:36:VAL:O	2.68	0.42
1:K:178:PHE:HE1	1:L:161:HIS:HE1	1.67	0.42
1:L:160:ILE:HG12	1:L:160:ILE:O	2.19	0.42
1:C:118:ARG:O	1:C:121:ILE:HD11	2.20	0.41
1:F:151:SER:OG	1:F:154:MET:HG3	2.20	0.41
1:G:113:LYS:NZ	1:H:108:VAL:O	2.53	0.41
1:G:229:ASP:O	1:G:236:PHE:HA	2.19	0.41
1:I:91:LEU:HA	1:I:91:LEU:HD23	1.78	0.41
1:K:37:VAL:CG1	1:K:90:LYS:HE2	2.50	0.41
1:K:149:GLY:O	1:K:191:SER:HA	2.18	0.41
1:L:238:MET:HE1	1:L:259:LEU:CD2	2.50	0.41
1:C:240:LYS:HE3	1:C:240:LYS:HB3	1.90	0.41
1:E:211:LEU:HA	1:E:214:ILE:HB	2.01	0.41
1:H:25:ALA:HB2	1:H:207:TRP:NE1	2.33	0.41
1:H:41:LEU:HD23	1:H:41:LEU:HA	1.81	0.41
1:J:247:LYS:HB2	1:J:247:LYS:HE2	1.36	0.41
1:K:126:TYR:CD1	1:K:126:TYR:C	2.93	0.41
1:B:235:GLY:O	1:F:153:SER:OG	2.37	0.41
1:D:189:THR:CG2	5:D:423:HOH:O	2.61	0.41
1:G:245:GLU:O	1:G:245:GLU:HG2	2.19	0.41
1:K:113:LYS:HD2	1:K:113:LYS:HA	1.84	0.41
1:D:127:THR:OG1	1:D:130:ALA:HB3	2.20	0.41
1:F:211:LEU:HA	1:F:214:ILE:HB	2.01	0.41
1:G:238:MET:HG2	1:G:242:VAL:CG1	2.51	0.41
1:G:259:LEU:HD23	1:G:259:LEU:HA	1.73	0.41
1:I:30:LYS:HE2	1:I:36:VAL:HG21	2.02	0.41
1:G:211:LEU:O	1:G:214:ILE:HG22	2.20	0.41
1:I:53:LYS:HA	1:I:53:LYS:HD2	1.74	0.41
1:J:244:ASP:HA	1:J:247:LYS:CD	2.28	0.41
1:L:230:LEU:HA	1:L:236:PHE:CD2	2.56	0.41
1:G:133:ASP:OD1	1:G:133:ASP:N	2.49	0.41
1:K:52:ARG:NH1	1:L:13:GLU:OE1	2.54	0.41
1:L:113:LYS:HA	1:L:113:LYS:HD2	1.93	0.41
1:C:54:ASP:OD2	1:C:118:ARG:HD2	2.21	0.41
1:A:123:GLU:HA	1:A:127:THR:HG22	2.03	0.41
1:B:117:GLU:OE2	1:F:109:PRO:HA	2.20	0.41
1:C:23:GLU:OE1	1:C:23:GLU:HA	2.19	0.41
1:C:155:TYR:HB3	1:C:164:MET:HB2	2.03	0.41
1:J:21:MET:SD	1:J:204:LEU:HD23	2.61	0.41
1:J:149:GLY:O	1:J:191:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:ILE:HD13	1:L:132:TYR:HE2	1.85	0.41
1:K:198:ASP:O	1:K:202:GLN:HG2	2.21	0.41
1:E:211:LEU:CD2	1:E:214:ILE:HD13	2.50	0.41
1:E:238:MET:O	1:E:243:GLN:NE2	2.51	0.41
1:G:83:ASP:OD1	1:G:83:ASP:N	2.54	0.41
1:H:40:ASP:O	1:H:44:MET:HG3	2.21	0.41
1:L:199:ALA:O	1:L:203:ILE:HG13	2.21	0.41
1:B:5:ALA:O	1:B:36:VAL:HA	2.21	0.40
1:L:55:ILE:HG23	1:L:74:ALA:HB2	2.04	0.40
1:D:36:VAL:O	1:D:36:VAL:CG2	2.68	0.40
1:J:3:ARG:HE	1:J:3:ARG:HB3	1.62	0.40
1:B:25:ALA:HA	1:B:211:LEU:CD1	2.51	0.40
1:D:261:LYS:CE	5:D:438:HOH:O	2.68	0.40
1:K:173:SER:HA	1:K:177:HIS:HB3	2.02	0.40
1:C:29:LEU:HB3	1:C:34:TRP:HB2	2.04	0.40
1:C:89:LYS:HA	1:C:89:LYS:HD2	1.89	0.40
1:E:29:LEU:CD1	1:E:211:LEU:HB3	2.51	0.40
1:F:9:LEU:CB	1:F:22:LYS:HE3	2.52	0.40
1:F:55:ILE:HD12	1:F:55:ILE:H	1.84	0.40
1:F:240:LYS:HB2	1:F:241:GLU:OE1	2.21	0.40
1:H:81:SER:HA	1:H:82:PRO:HD3	1.93	0.40
1:B:36:VAL:HG22	1:B:36:VAL:O	2.21	0.40
1:C:148:THR:OG1	1:C:190:TYR:HA	2.21	0.40
1:D:130:ALA:O	1:D:135:GLY:HA2	2.22	0.40
1:F:153:SER:O	1:F:159:GLY:HA3	2.22	0.40
1:G:230:LEU:HD22	1:H:160:ILE:HD12	2.01	0.40
1:H:122:GLY:O	1:H:123:GLU:HB2	2.20	0.40
1:I:7:ILE:HG21	1:I:22:LYS:HG2	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:MET:CE	3:E:2302:EHL:O1[4_654]	1.37	0.83
1:C:131:MET:CE	3:E:2302:EHL:N2[4_654]	1.49	0.71
1:C:131:MET:CE	3:E:2302:EHL:O2[4_654]	2.12	0.08
1:C:262:SER:OG	1:E:260:GLY:O[4_654]	2.17	0.03

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	270/273 (99%)	256 (95%)	14 (5%)	0	100	100
1	B	269/273 (98%)	250 (93%)	19 (7%)	0	100	100
1	C	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
1	D	270/273 (99%)	257 (95%)	13 (5%)	0	100	100
1	E	269/273 (98%)	254 (94%)	15 (6%)	0	100	100
1	F	269/273 (98%)	247 (92%)	22 (8%)	0	100	100
1	G	268/273 (98%)	253 (94%)	15 (6%)	0	100	100
1	H	268/273 (98%)	249 (93%)	19 (7%)	0	100	100
1	I	268/273 (98%)	254 (95%)	14 (5%)	0	100	100
1	J	268/273 (98%)	254 (95%)	13 (5%)	1 (0%)	34	54
1	K	269/273 (98%)	250 (93%)	18 (7%)	1 (0%)	34	54
1	L	269/273 (98%)	250 (93%)	19 (7%)	0	100	100
All	All	3226/3276 (98%)	3032 (94%)	192 (6%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	60	LYS
1	J	40	ASP

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	226/227 (100%)	217 (96%)	9 (4%)	31	56
1	B	225/227 (99%)	219 (97%)	6 (3%)	44	71
1	C	225/227 (99%)	219 (97%)	6 (3%)	44	71
1	D	226/227 (100%)	219 (97%)	7 (3%)	40	67
1	E	225/227 (99%)	220 (98%)	5 (2%)	52	77
1	F	225/227 (99%)	219 (97%)	6 (3%)	44	71
1	G	225/227 (99%)	220 (98%)	5 (2%)	52	77
1	H	225/227 (99%)	217 (96%)	8 (4%)	35	61
1	I	225/227 (99%)	220 (98%)	5 (2%)	52	77
1	J	225/227 (99%)	219 (97%)	6 (3%)	44	71
1	K	225/227 (99%)	212 (94%)	13 (6%)	20	38
1	L	225/227 (99%)	223 (99%)	2 (1%)	78	92
All	All	2702/2724 (99%)	2624 (97%)	78 (3%)	42	69

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	29	LEU
1	A	36	VAL
1	A	56	THR
1	A	91	LEU
1	A	92	GLU
1	A	189	THR
1	A	214	ILE
1	A	254	SER
1	B	22	LYS
1	B	23	GLU
1	B	29	LEU
1	B	36	VAL
1	B	52	ARG
1	B	173	SER
1	C	15	THR
1	C	29	LEU
1	C	92	GLU
1	C	158	GLN
1	C	189	THR
1	C	232	PHE
1	D	36	VAL

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Mol	Chain	Res	Type
1	D	52	ARG
1	D	60	LYS
1	D	92	GLU
1	D	127	THR
1	D	189	THR
1	D	238	MET
1	E	29	LEU
1	E	89	LYS
1	E	128	TYR
1	E	232	PHE
1	E	238	MET
1	F	29	LEU
1	F	60	LYS
1	F	89	LYS
1	F	92	GLU
1	F	131	MET
1	F	241	GLU
1	G	22	LYS
1	G	36	VAL
1	G	89	LYS
1	G	189	THR
1	G	214	ILE
1	H	22	LYS
1	H	29	LEU
1	H	139	SER
1	H	189	THR
1	H	191	SER
1	H	194	HIS
1	H	238	MET
1	H	262	SER
1	I	14	ARG
1	I	53	LYS
1	I	92	GLU
1	I	227	LEU
1	I	233	GLN
1	J	35	GLU
1	J	52	ARG
1	J	92	GLU
1	J	153	SER
1	J	160	ILE
1	J	213	ASN
1	K	14	ARG

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Mol	Chain	Res	Type
1	K	29	LEU
1	K	36	VAL
1	K	39	SER
1	K	58	LYS
1	K	64	ASN
1	K	92	GLU
1	K	112	LEU
1	K	128	TYR
1	K	160	ILE
1	K	189	THR
1	K	226	SER
1	K	238	MET
1	L	22	LYS
1	L	39	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	45	ASN
1	G	45	ASN
1	L	79	HIS

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)

24 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	F	2301	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
2	FAD	J	302	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
3	EHL	H	301	-	19,25,25	4.74	10 (52%)	15,35,35	2.74	4 (26%)
2	FAD	K	2301	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
2	FAD	E	2301	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
3	EHL	D	301	-	19,25,25	4.76	10 (52%)	15,35,35	2.97	3 (20%)
4	SO4	J	303	-	4,4,4	0.29	0	6,6,6	0.31	0
2	FAD	C	2301	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
2	FAD	I	2301	-	53,58,58	0.44	0	68,89,89	0.55	2 (2%)
3	EHL	A	2302	-	19,25,25	4.75	10 (52%)	15,35,35	2.14	4 (26%)
4	SO4	A	2303	-	4,4,4	0.26	0	6,6,6	0.27	0
3	EHL	B	2302	-	19,25,25	4.86	10 (52%)	15,35,35	2.32	4 (26%)
2	FAD	G	2301	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
3	EHL	J	301	-	19,25,25	4.82	10 (52%)	15,35,35	2.05	4 (26%)
3	EHL	E	2302	-	19,25,25	4.78	10 (52%)	15,35,35	2.29	4 (26%)
4	SO4	D	303	-	4,4,4	0.39	0	6,6,6	0.46	0
2	FAD	D	302	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
2	FAD	H	302	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
3	EHL	I	2302	-	19,25,25	4.81	10 (52%)	15,35,35	1.77	3 (20%)
2	FAD	A	2301	-	53,58,58	0.48	0	68,89,89	0.59	3 (4%)
2	FAD	L	302	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
4	SO4	F	2302	-	4,4,4	0.21	0	6,6,6	0.17	0
2	FAD	B	2301	-	53,58,58	0.45	0	68,89,89	0.55	2 (2%)
3	EHL	L	301	-	19,25,25	4.66	10 (52%)	15,35,35	2.10	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	F	2301	-	-	4/30/50/50	0/6/6/6
2	FAD	J	302	-	-	4/30/50/50	0/6/6/6
3	EHL	H	301	-	-	2/6/16/16	0/3/3/3
2	FAD	K	2301	-	-	4/30/50/50	0/6/6/6
2	FAD	E	2301	-	-	5/30/50/50	0/6/6/6
3	EHL	D	301	-	-	2/6/16/16	0/3/3/3
2	FAD	C	2301	-	-	4/30/50/50	0/6/6/6
2	FAD	I	2301	-	-	4/30/50/50	0/6/6/6
3	EHL	A	2302	-	-	2/6/16/16	0/3/3/3
3	EHL	B	2302	-	-	2/6/16/16	0/3/3/3
2	FAD	G	2301	-	-	4/30/50/50	0/6/6/6
3	EHL	J	301	-	-	2/6/16/16	0/3/3/3
3	EHL	E	2302	-	-	2/6/16/16	0/3/3/3
2	FAD	D	302	-	-	4/30/50/50	0/6/6/6
2	FAD	H	302	-	-	4/30/50/50	0/6/6/6
3	EHL	I	2302	-	-	2/6/16/16	0/3/3/3
2	FAD	A	2301	-	-	4/30/50/50	0/6/6/6
2	FAD	L	302	-	-	4/30/50/50	0/6/6/6
2	FAD	B	2301	-	-	5/30/50/50	0/6/6/6
3	EHL	L	301	-	-	2/6/16/16	0/3/3/3

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2302	EHL	C2-C3	15.72	1.56	1.38
3	J	301	EHL	C2-C3	15.71	1.56	1.38
3	E	2302	EHL	C2-C3	15.43	1.56	1.38
3	A	2302	EHL	C2-C3	15.39	1.56	1.38
3	I	2302	EHL	C2-C3	15.30	1.56	1.38
3	H	301	EHL	C2-C3	15.26	1.55	1.38
3	D	301	EHL	C2-C3	15.10	1.55	1.38
3	L	301	EHL	C2-C3	15.03	1.55	1.38
3	I	2302	EHL	C2-N1	9.69	1.50	1.36
3	B	2302	EHL	C2-N1	9.68	1.50	1.36
3	J	301	EHL	C2-N1	9.63	1.50	1.36
3	E	2302	EHL	C2-N1	9.62	1.50	1.36
3	A	2302	EHL	C2-N1	9.49	1.50	1.36
3	D	301	EHL	C2-N1	9.22	1.49	1.36
3	L	301	EHL	C2-N1	9.06	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	EHL	C2-N1	8.81	1.49	1.36
3	D	301	EHL	C1-N	6.03	1.47	1.36
3	H	301	EHL	C1-N	5.81	1.46	1.36
3	B	2302	EHL	C1-N	5.67	1.46	1.36
3	E	2302	EHL	C1-N	5.61	1.46	1.36
3	I	2302	EHL	C1-N	5.51	1.46	1.36
3	J	301	EHL	C1-N	5.36	1.46	1.36
3	L	301	EHL	C1-N	5.31	1.46	1.36
3	A	2302	EHL	C1-N	5.17	1.45	1.36
3	H	301	EHL	C-N	4.21	1.46	1.35
3	D	301	EHL	C-N	4.13	1.46	1.35
3	I	2302	EHL	C-N	3.96	1.46	1.35
3	E	2302	EHL	C-N	3.90	1.46	1.35
3	B	2302	EHL	C-N	3.89	1.46	1.35
3	L	301	EHL	C-N	3.88	1.46	1.35
3	I	2302	EHL	C8-C7	3.75	1.53	1.49
3	J	301	EHL	C-N	3.72	1.45	1.35
3	H	301	EHL	C3-S	3.68	1.81	1.74
3	A	2302	EHL	C8-C7	3.66	1.53	1.49
3	D	301	EHL	C4-C7	3.63	1.45	1.41
3	D	301	EHL	C8-C7	3.59	1.53	1.49
3	A	2302	EHL	C-N	3.59	1.45	1.35
3	L	301	EHL	C6-C5	3.54	1.53	1.48
3	H	301	EHL	C6-C5	3.54	1.53	1.48
3	I	2302	EHL	C4-C7	3.52	1.45	1.41
3	D	301	EHL	C6-C5	3.48	1.53	1.48
3	A	2302	EHL	C6-C5	3.47	1.53	1.48
3	E	2302	EHL	C6-C5	3.43	1.53	1.48
3	B	2302	EHL	C8-C7	3.41	1.53	1.49
3	J	301	EHL	C6-C5	3.41	1.53	1.48
3	L	301	EHL	C3-S	3.40	1.80	1.74
3	L	301	EHL	C8-C7	3.36	1.52	1.49
3	B	2302	EHL	C6-C5	3.35	1.53	1.48
3	J	301	EHL	C8-C7	3.35	1.52	1.49
3	I	2302	EHL	C6-C5	3.34	1.53	1.48
3	H	301	EHL	C8-C7	3.31	1.52	1.49
3	E	2302	EHL	C3-S	3.20	1.80	1.74
3	B	2302	EHL	C3-S	3.16	1.80	1.74
3	E	2302	EHL	C8-C7	3.13	1.52	1.49
3	J	301	EHL	O1-N2	-3.05	1.17	1.22
3	J	301	EHL	C3-S	3.05	1.80	1.74
3	L	301	EHL	O1-N2	-3.04	1.17	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2302	EHL	O1-N2	-3.03	1.17	1.22
3	A	2302	EHL	C3-S	2.99	1.79	1.74
3	H	301	EHL	O1-N2	-2.99	1.17	1.22
3	H	301	EHL	C4-C7	2.94	1.44	1.41
3	D	301	EHL	C3-S	2.93	1.79	1.74
3	I	2302	EHL	C3-S	2.91	1.79	1.74
3	I	2302	EHL	O1-N2	-2.91	1.17	1.22
3	B	2302	EHL	C4-C7	2.90	1.44	1.41
3	A	2302	EHL	C4-C7	2.89	1.44	1.41
3	B	2302	EHL	O1-N2	-2.86	1.17	1.22
3	E	2302	EHL	O1-N2	-2.81	1.18	1.22
3	J	301	EHL	C4-C7	2.81	1.44	1.41
3	L	301	EHL	C4-C7	2.65	1.44	1.41
3	E	2302	EHL	C4-C7	2.59	1.44	1.41
3	B	2302	EHL	O-C	-2.41	1.18	1.23
3	A	2302	EHL	O-C	-2.39	1.18	1.23
3	I	2302	EHL	O-C	-2.35	1.18	1.23
3	E	2302	EHL	O-C	-2.35	1.18	1.23
3	D	301	EHL	O1-N2	-2.34	1.18	1.22
3	J	301	EHL	O-C	-2.34	1.18	1.23
3	H	301	EHL	O-C	-2.29	1.18	1.23
3	L	301	EHL	O-C	-2.27	1.18	1.23
3	D	301	EHL	O-C	-2.23	1.18	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	301	EHL	C2-C3-N2	-10.21	118.97	126.98
3	H	301	EHL	C2-C3-N2	-8.30	120.47	126.98
3	E	2302	EHL	C2-C3-N2	-5.65	122.54	126.98
3	B	2302	EHL	C2-C3-N2	-5.46	122.69	126.98
3	L	301	EHL	C2-C3-N2	-5.05	123.02	126.98
3	B	2302	EHL	C4-C-N	4.81	123.95	114.91
3	A	2302	EHL	C2-C3-N2	-4.59	123.38	126.98
3	E	2302	EHL	C4-C-N	4.48	123.34	114.91
3	A	2302	EHL	C4-C-N	4.40	123.18	114.91
3	H	301	EHL	C4-C-N	4.37	123.12	114.91
3	J	301	EHL	C4-C-N	4.34	123.08	114.91
3	J	301	EHL	C2-C3-N2	-4.15	123.72	126.98
3	I	2302	EHL	C2-C3-N2	-3.93	123.89	126.98
3	L	301	EHL	C4-C-N	3.92	122.28	114.91
3	A	2302	EHL	C1-N-C	-3.90	116.97	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	301	EHL	C4-C-N	3.90	122.25	114.91
3	J	301	EHL	C1-N-C	-3.70	117.49	126.64
3	I	2302	EHL	C4-C-N	3.69	121.84	114.91
3	L	301	EHL	C1-N-C	-3.47	118.04	126.64
3	B	2302	EHL	C1-N-C	-3.39	118.24	126.64
3	E	2302	EHL	C1-N-C	-3.22	118.68	126.64
3	H	301	EHL	C1-N-C	-3.01	119.18	126.64
3	I	2302	EHL	C1-N-C	-2.91	119.44	126.64
3	H	301	EHL	O-C-C4	-2.80	116.74	120.95
3	B	2302	EHL	O-C-C4	-2.74	116.82	120.95
3	E	2302	EHL	O-C-C4	-2.73	116.84	120.95
2	B	2301	FAD	P-O3P-PA	-2.56	124.05	132.83
2	C	2301	FAD	P-O3P-PA	-2.54	124.12	132.83
2	E	2301	FAD	P-O3P-PA	-2.53	124.16	132.83
2	K	2301	FAD	P-O3P-PA	-2.51	124.20	132.83
2	G	2301	FAD	P-O3P-PA	-2.51	124.21	132.83
2	L	302	FAD	P-O3P-PA	-2.50	124.26	132.83
2	F	2301	FAD	P-O3P-PA	-2.49	124.28	132.83
2	J	302	FAD	P-O3P-PA	-2.48	124.30	132.83
2	D	302	FAD	P-O3P-PA	-2.48	124.31	132.83
2	H	302	FAD	P-O3P-PA	-2.48	124.32	132.83
2	I	2301	FAD	P-O3P-PA	-2.46	124.37	132.83
3	D	301	EHL	O-C-C4	-2.44	117.28	120.95
2	A	2301	FAD	P-O3P-PA	-2.43	124.50	132.83
3	A	2302	EHL	O-C-N	-2.41	118.21	123.71
3	L	301	EHL	O-C-C4	-2.38	117.37	120.95
2	C	2301	FAD	C5A-C6A-N6A	2.31	123.86	120.35
2	H	302	FAD	C5A-C6A-N6A	2.30	123.85	120.35
2	K	2301	FAD	C5A-C6A-N6A	2.29	123.83	120.35
2	D	302	FAD	C5A-C6A-N6A	2.29	123.83	120.35
2	G	2301	FAD	C5A-C6A-N6A	2.28	123.82	120.35
2	F	2301	FAD	C5A-C6A-N6A	2.28	123.81	120.35
2	E	2301	FAD	C5A-C6A-N6A	2.27	123.80	120.35
2	B	2301	FAD	C5A-C6A-N6A	2.27	123.80	120.35
2	L	302	FAD	C5A-C6A-N6A	2.27	123.80	120.35
2	I	2301	FAD	C5A-C6A-N6A	2.26	123.79	120.35
2	J	302	FAD	C5A-C6A-N6A	2.26	123.78	120.35
2	A	2301	FAD	C5A-C6A-N6A	2.17	123.65	120.35
2	A	2301	FAD	C4A-C5A-N7A	2.17	111.66	109.40
3	J	301	EHL	O-C-N	-2.11	118.88	123.71

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2302	EHL	N3-C7-C8-C9
3	A	2302	EHL	N3-C7-C8-C13
3	B	2302	EHL	N3-C7-C8-C9
3	B	2302	EHL	N3-C7-C8-C13
3	D	301	EHL	N3-C7-C8-C9
3	D	301	EHL	N3-C7-C8-C13
3	E	2302	EHL	N3-C7-C8-C9
3	H	301	EHL	N3-C7-C8-C9
3	H	301	EHL	N3-C7-C8-C13
3	J	301	EHL	N3-C7-C8-C9
3	J	301	EHL	N3-C7-C8-C13
3	L	301	EHL	N3-C7-C8-C9
3	L	301	EHL	N3-C7-C8-C13
3	E	2302	EHL	N3-C7-C8-C13
2	B	2301	FAD	O4B-C4B-C5B-O5B
2	D	302	FAD	O4B-C4B-C5B-O5B
2	F	2301	FAD	O4B-C4B-C5B-O5B
2	G	2301	FAD	O4B-C4B-C5B-O5B
2	H	302	FAD	O4B-C4B-C5B-O5B
2	I	2301	FAD	O4B-C4B-C5B-O5B
2	J	302	FAD	O4B-C4B-C5B-O5B
2	C	2301	FAD	O4B-C4B-C5B-O5B
2	E	2301	FAD	O4B-C4B-C5B-O5B
2	L	302	FAD	O4B-C4B-C5B-O5B
2	B	2301	FAD	O4'-C4'-C5'-O5'
2	K	2301	FAD	O4B-C4B-C5B-O5B
2	D	302	FAD	C3B-C4B-C5B-O5B
2	I	2301	FAD	C3B-C4B-C5B-O5B
2	C	2301	FAD	O4'-C4'-C5'-O5'
2	D	302	FAD	O4'-C4'-C5'-O5'
2	E	2301	FAD	O4'-C4'-C5'-O5'
2	F	2301	FAD	O4'-C4'-C5'-O5'
2	G	2301	FAD	O4'-C4'-C5'-O5'
2	H	302	FAD	O4'-C4'-C5'-O5'
2	I	2301	FAD	O4'-C4'-C5'-O5'
2	J	302	FAD	O4'-C4'-C5'-O5'
2	K	2301	FAD	O4'-C4'-C5'-O5'
2	L	302	FAD	O4'-C4'-C5'-O5'
3	I	2302	EHL	N3-C7-C8-C9
2	B	2301	FAD	C3B-C4B-C5B-O5B
2	F	2301	FAD	C3B-C4B-C5B-O5B
2	G	2301	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	H	302	FAD	C3B-C4B-C5B-O5B
2	J	302	FAD	C3B-C4B-C5B-O5B
2	A	2301	FAD	P-O3P-PA-O1A
2	A	2301	FAD	P-O3P-PA-O2A
2	C	2301	FAD	C3B-C4B-C5B-O5B
2	L	302	FAD	C3B-C4B-C5B-O5B
2	E	2301	FAD	C3B-C4B-C5B-O5B
2	K	2301	FAD	C3B-C4B-C5B-O5B
3	I	2302	EHL	N3-C7-C8-C13
2	A	2301	FAD	C5'-O5'-P-O3P
2	B	2301	FAD	C5'-O5'-P-O3P
2	E	2301	FAD	PA-O3P-P-O2P
2	A	2301	FAD	C5'-O5'-P-O1P
2	B	2301	FAD	C5B-O5B-PA-O1A
2	C	2301	FAD	C5B-O5B-PA-O1A
2	D	302	FAD	C5B-O5B-PA-O1A
2	E	2301	FAD	C5B-O5B-PA-O1A
2	F	2301	FAD	C5B-O5B-PA-O1A
2	G	2301	FAD	C5B-O5B-PA-O1A
2	H	302	FAD	C5B-O5B-PA-O1A
2	I	2301	FAD	C5B-O5B-PA-O1A
2	J	302	FAD	C5B-O5B-PA-O1A
2	K	2301	FAD	C5B-O5B-PA-O1A
2	L	302	FAD	C5B-O5B-PA-O1A

There are no ring outliers.

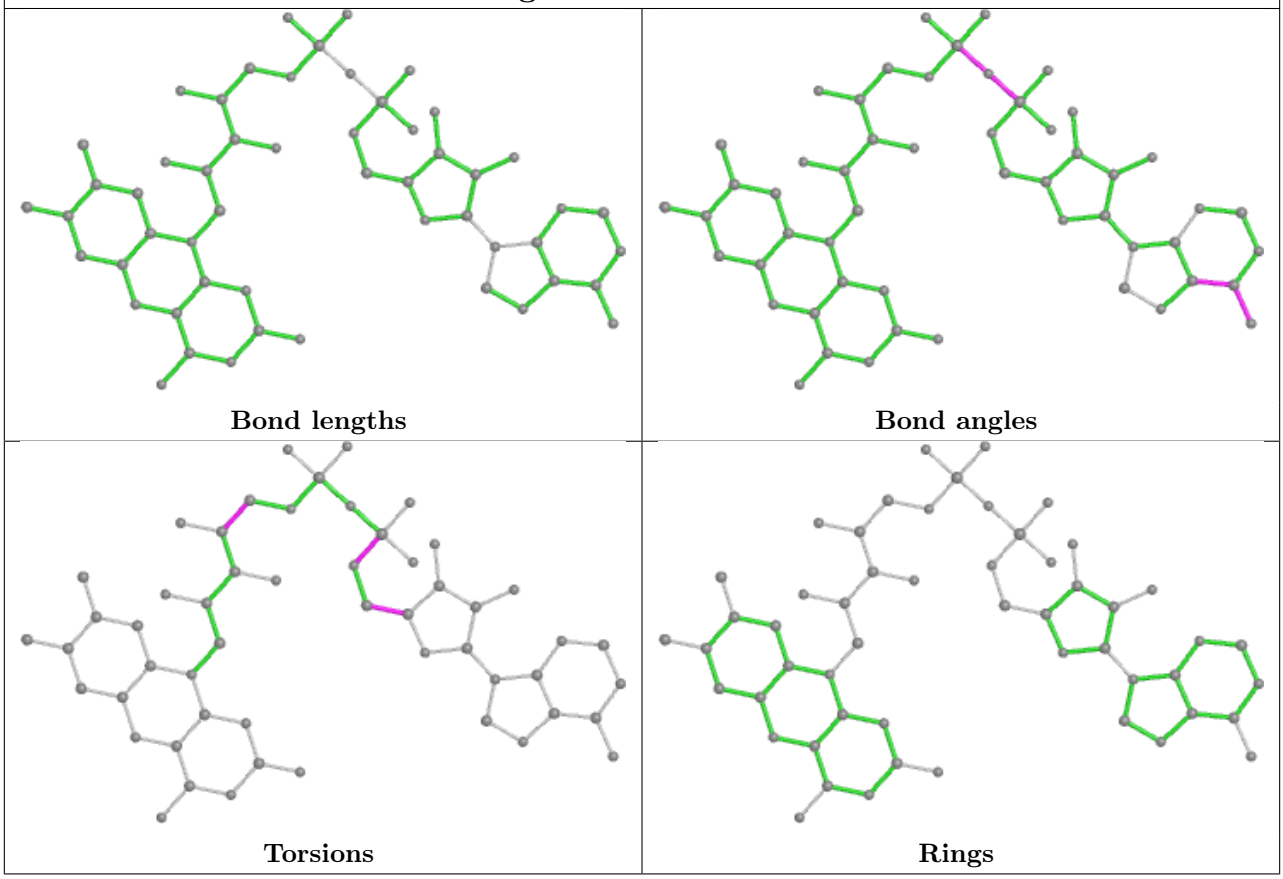
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	303	SO4	1	0
4	A	2303	SO4	1	0
3	E	2302	EHL	0	3
4	D	303	SO4	1	0

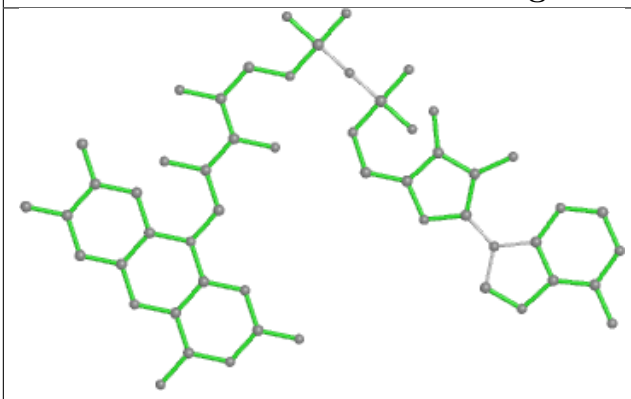
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

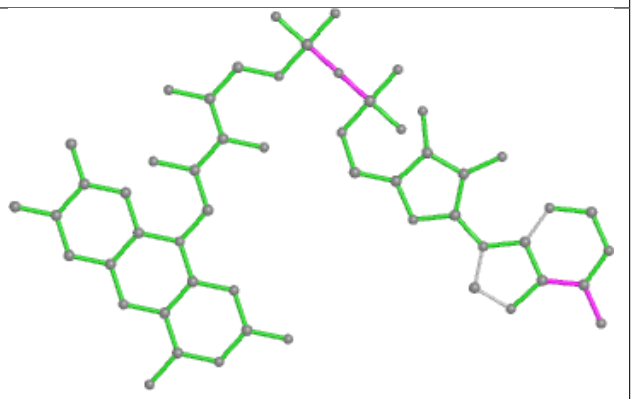
Ligand FAD F 2301



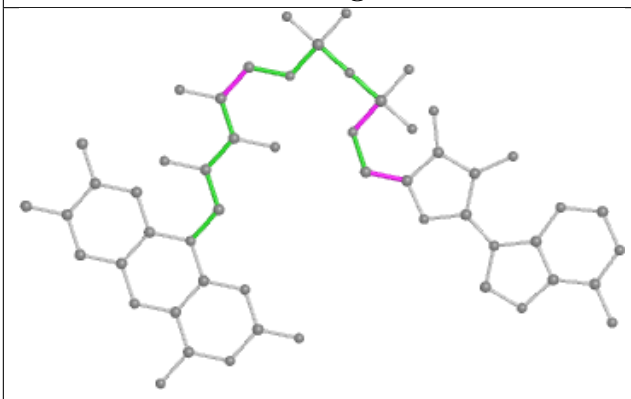
Ligand FAD J 302



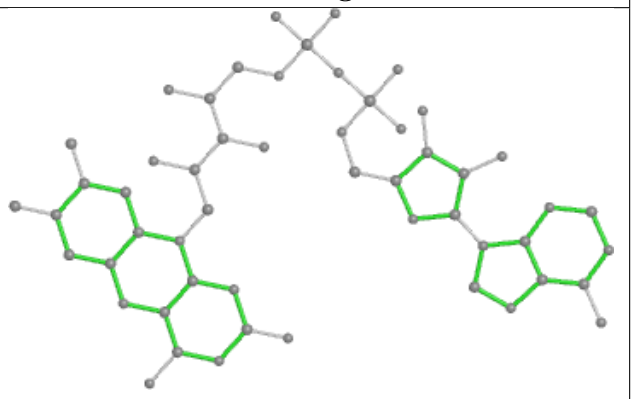
Bond lengths



Bond angles

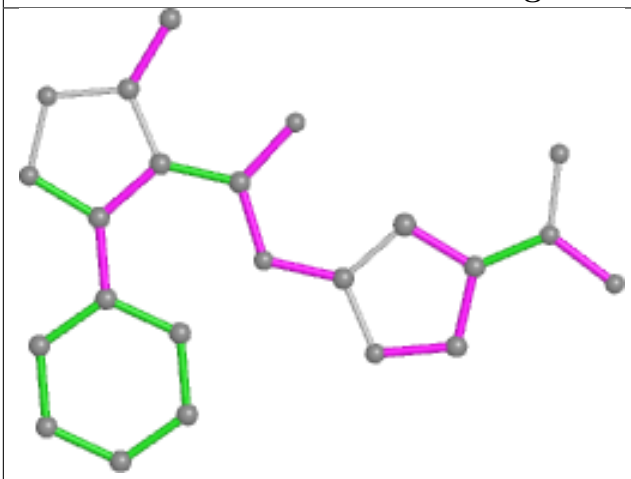


Torsions



Rings

Ligand EHL H 301



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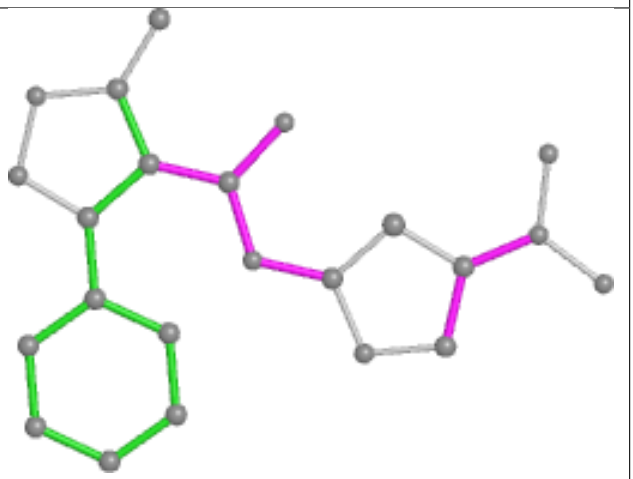

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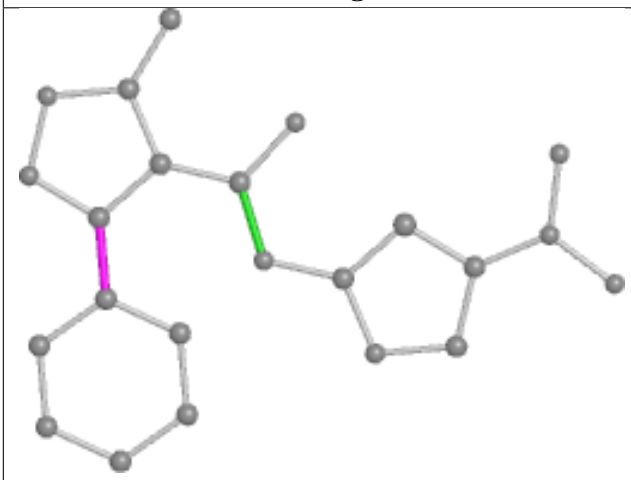

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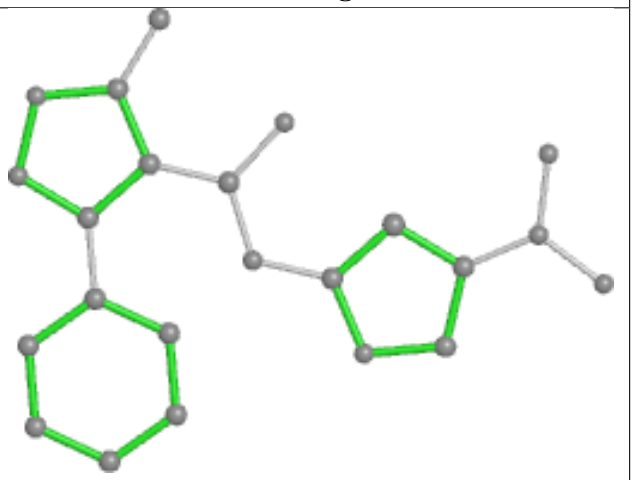
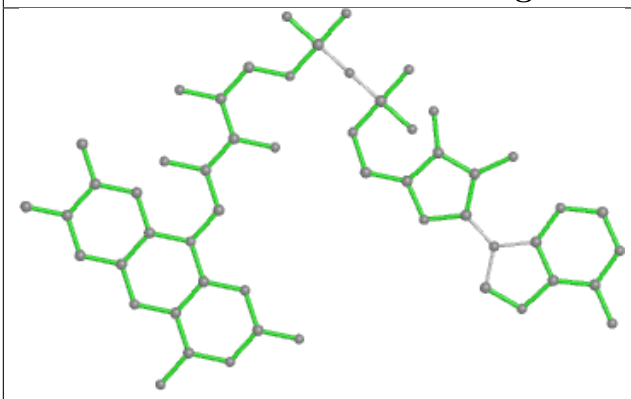


Rings

Ligand FAD K 2301



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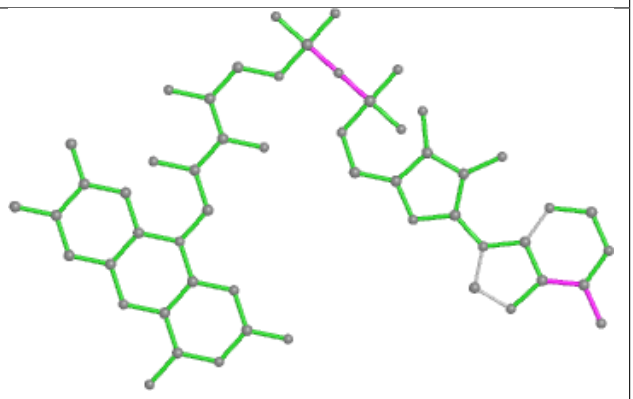

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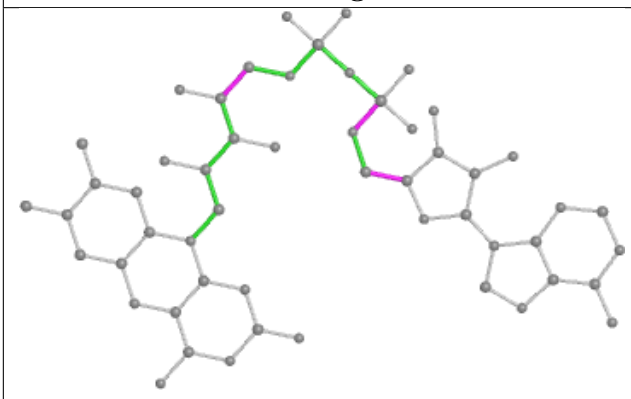

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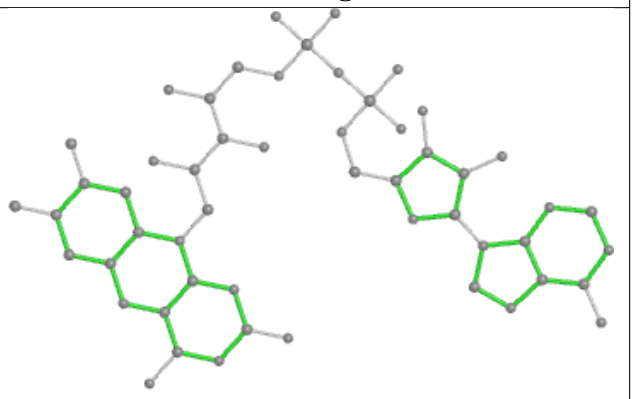
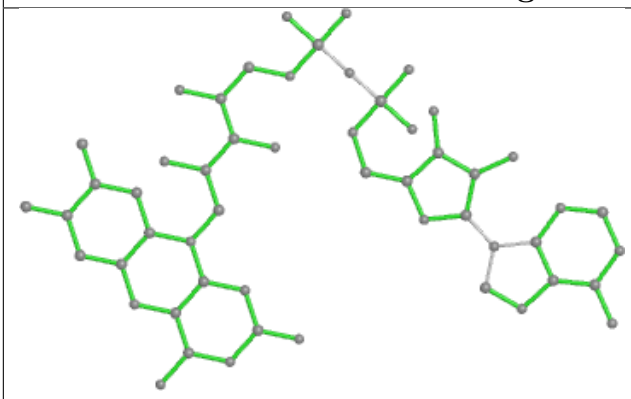


Rings

Ligand FAD E 2301



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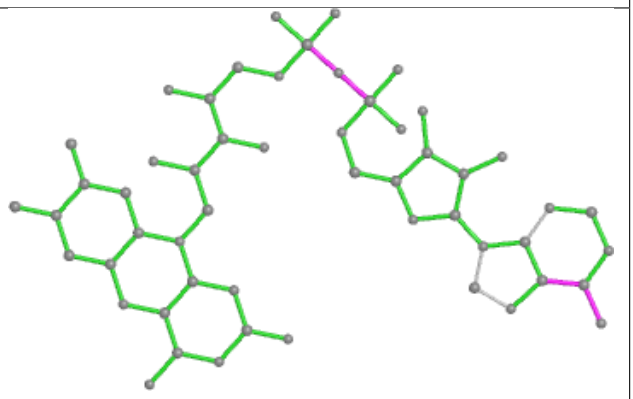

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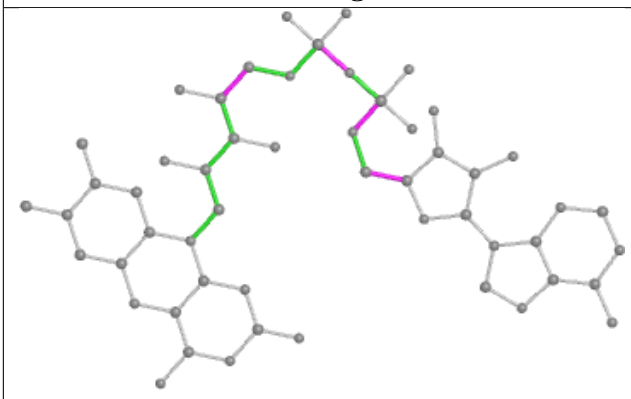

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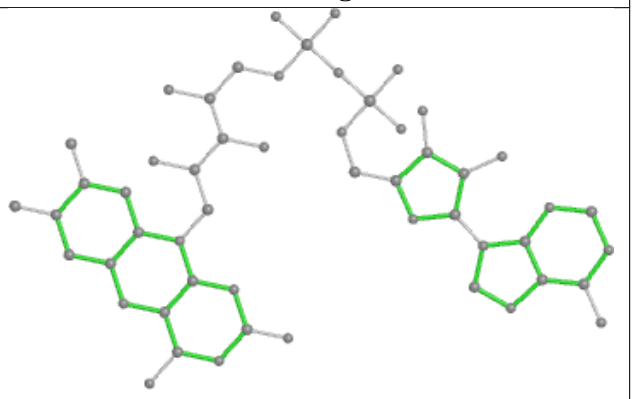
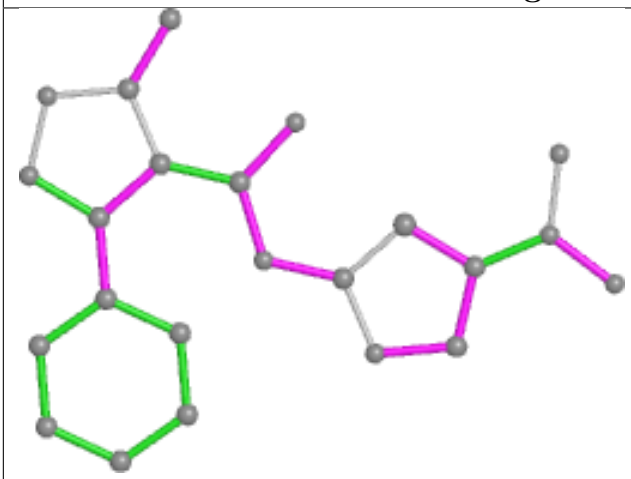


Rings

Ligand EHL D 301



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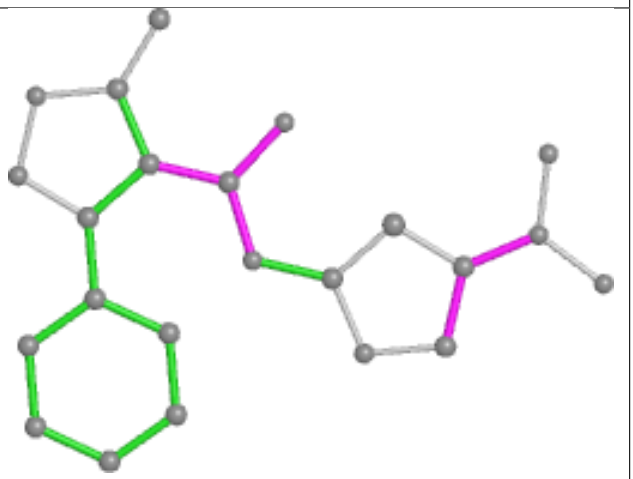

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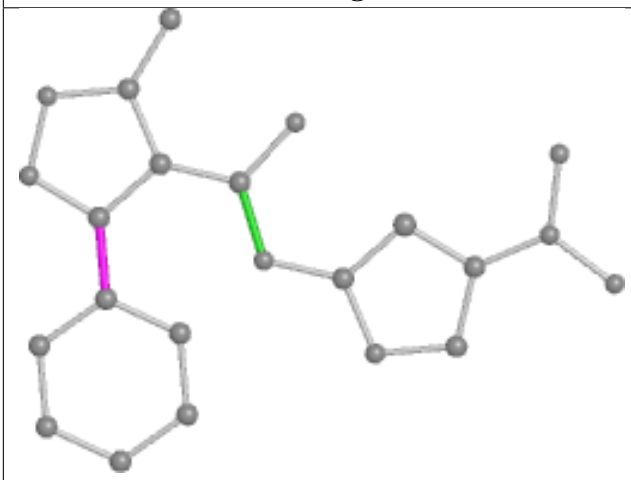

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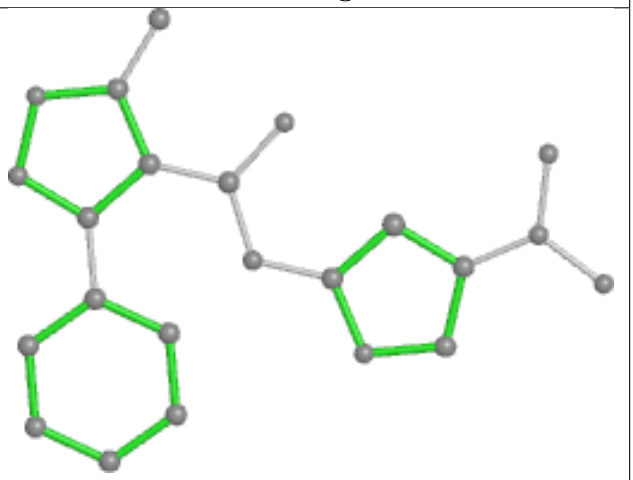
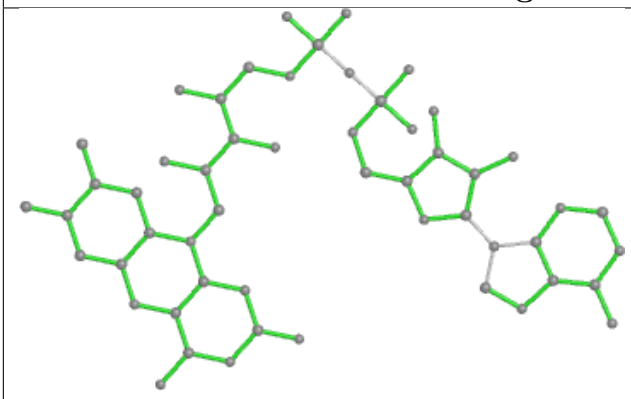


Rings

Ligand FAD C 2301



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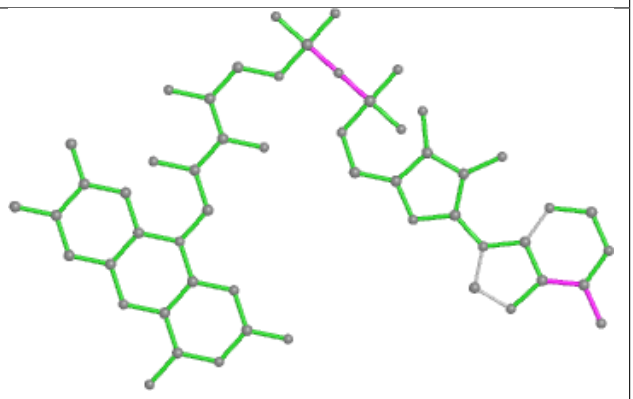

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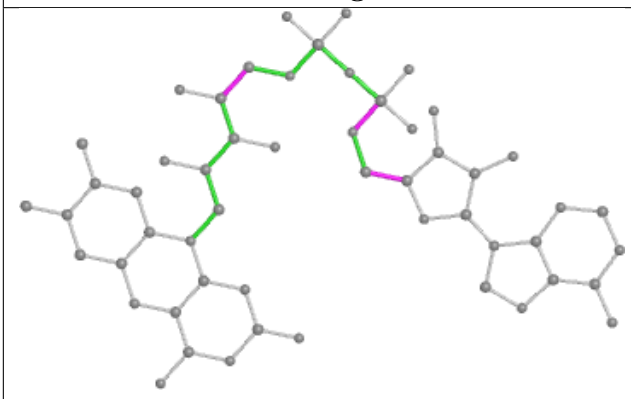

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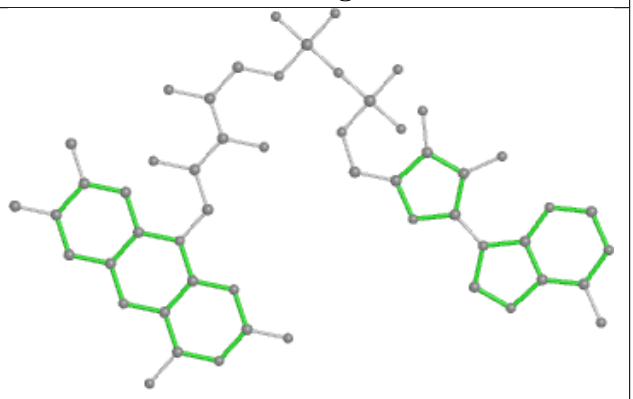
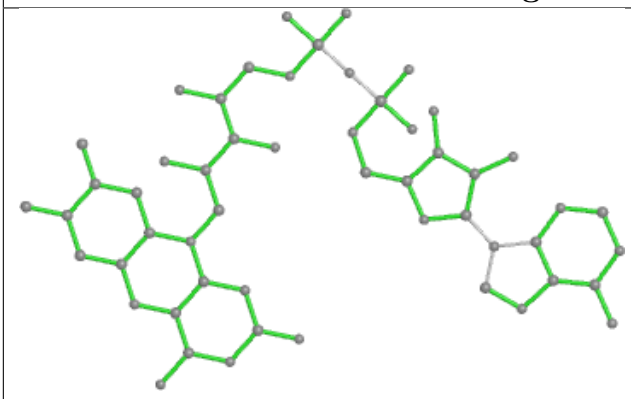


Rings

Ligand FAD I 2301



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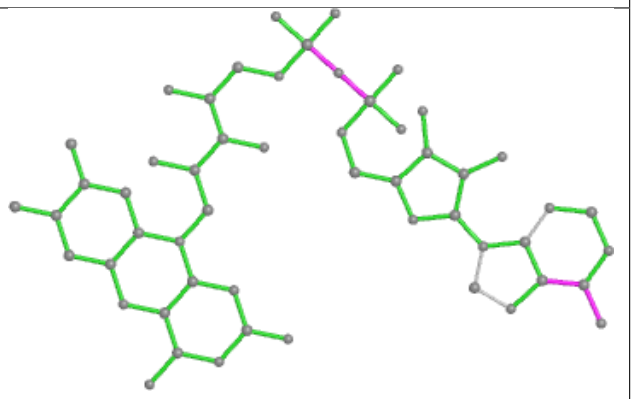

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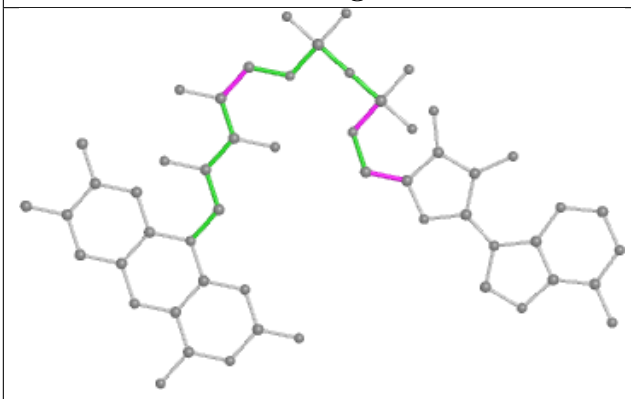

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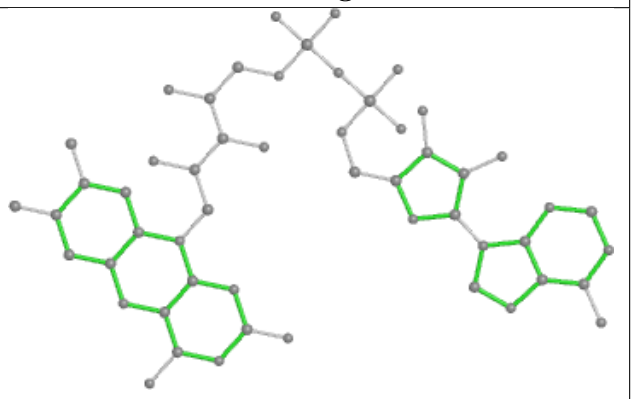
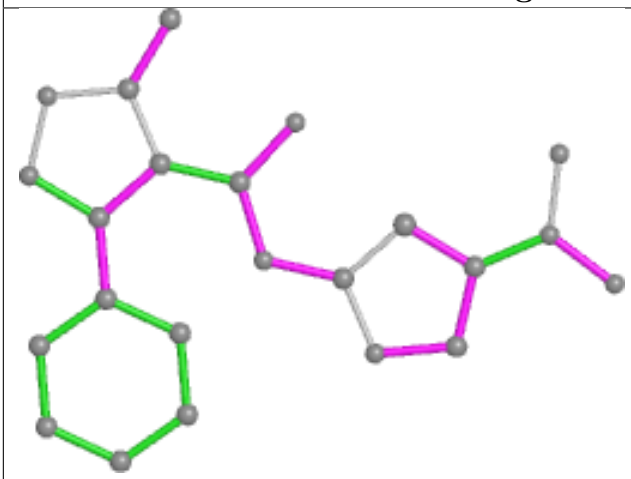


Rings

Ligand EHL A 2302



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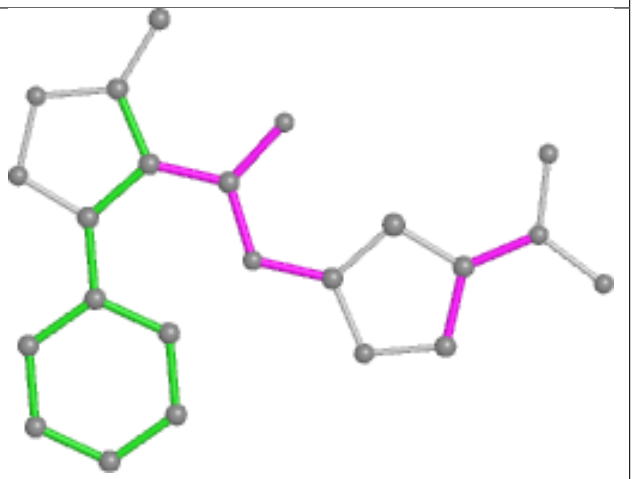

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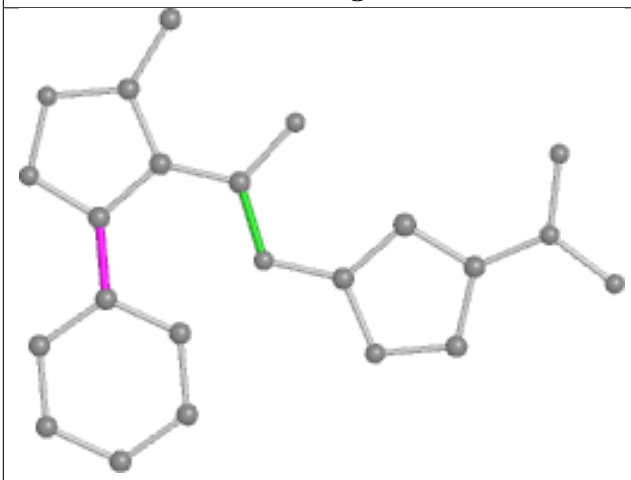

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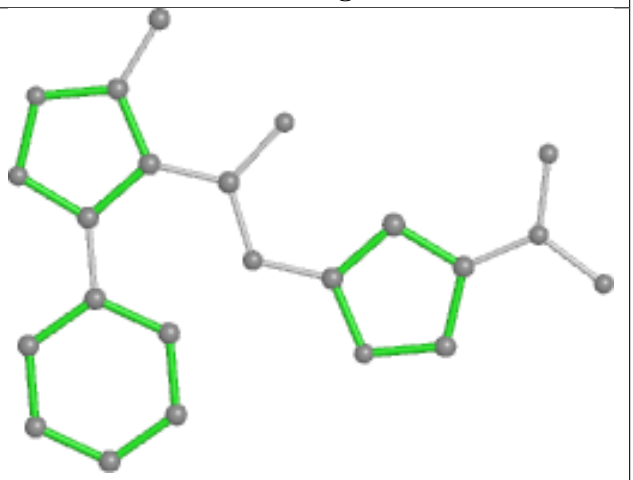
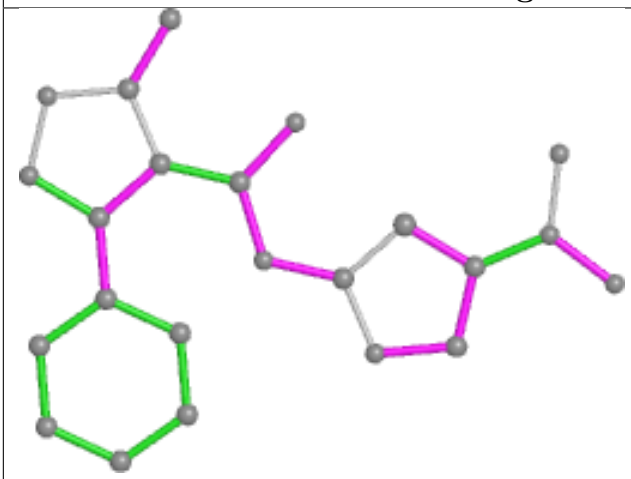


Rings

Ligand EHL B 2302



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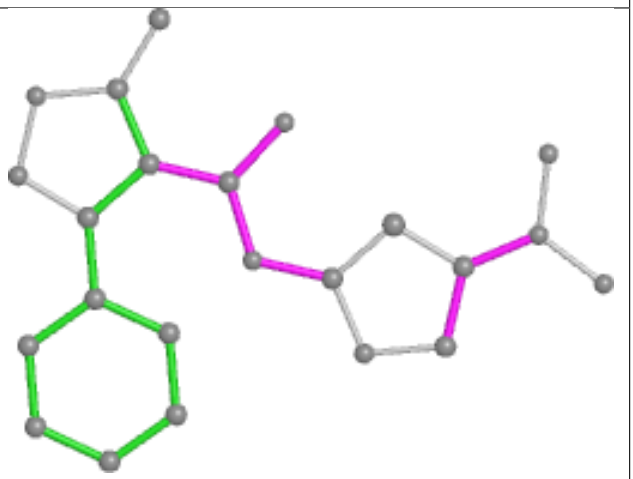

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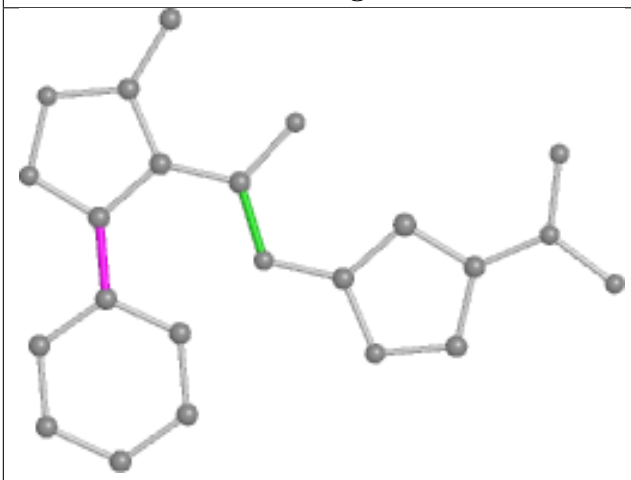

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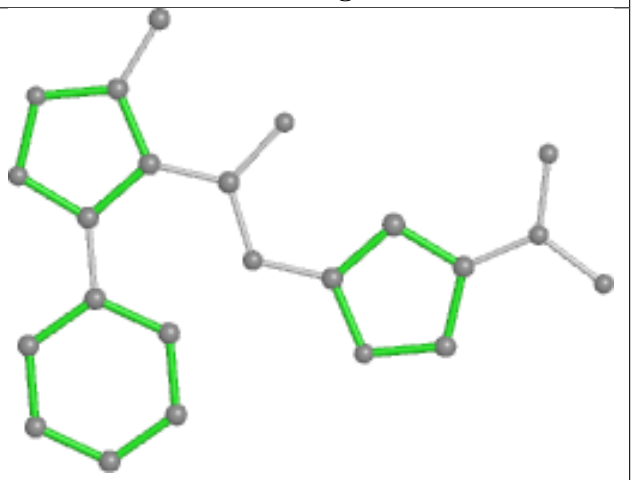
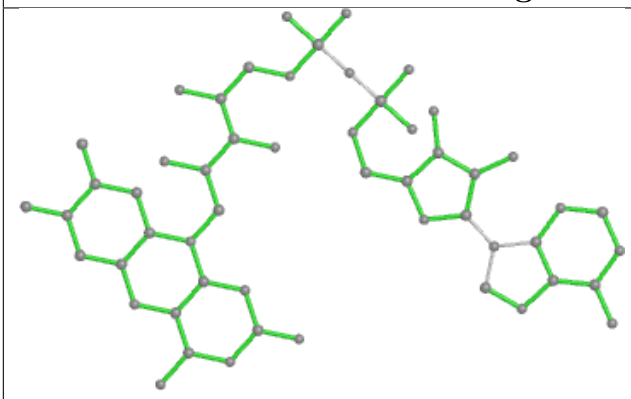


Rings

Ligand FAD G 2301



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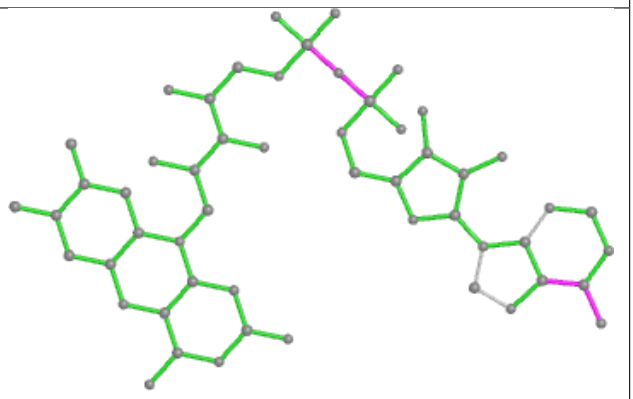

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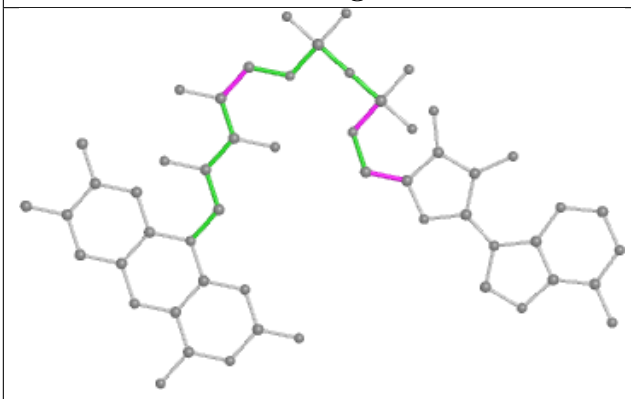

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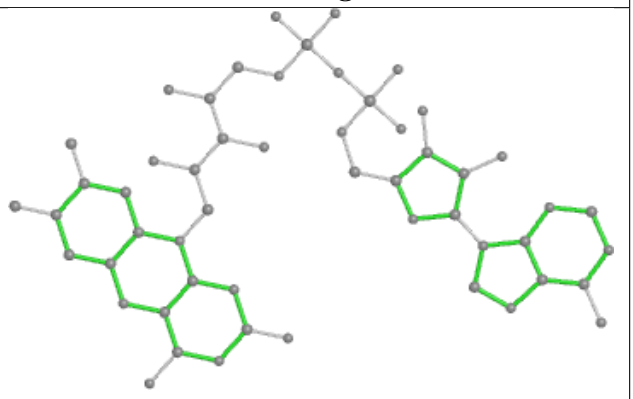
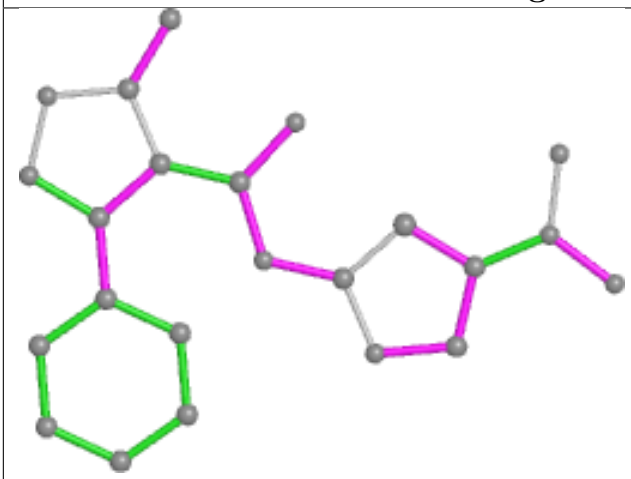


Rings

Ligand EHL J 301



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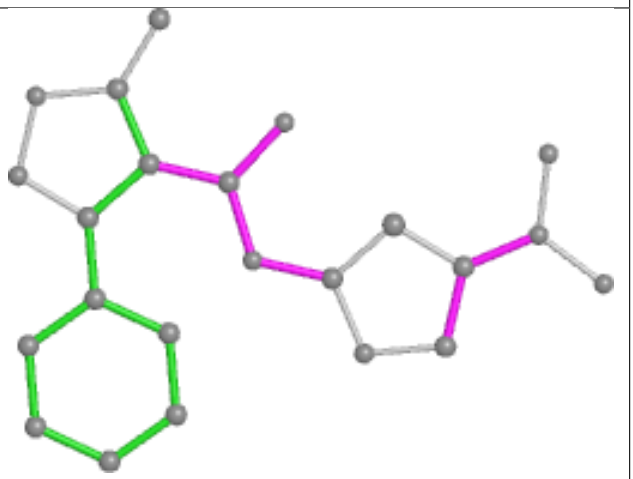

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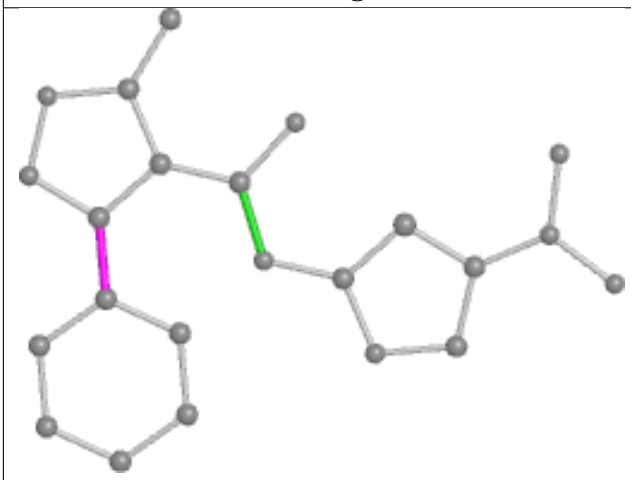

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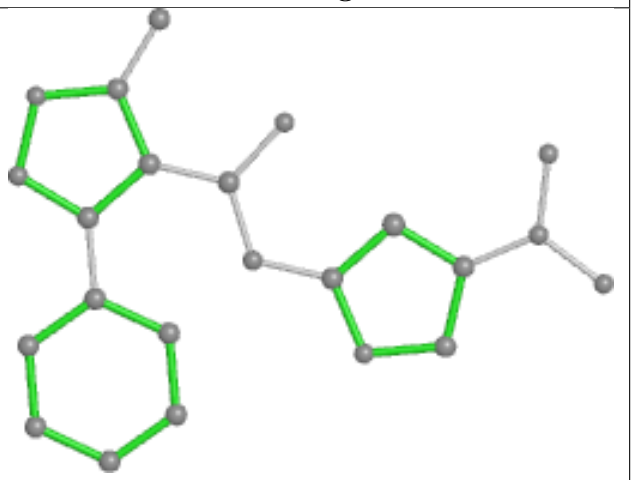
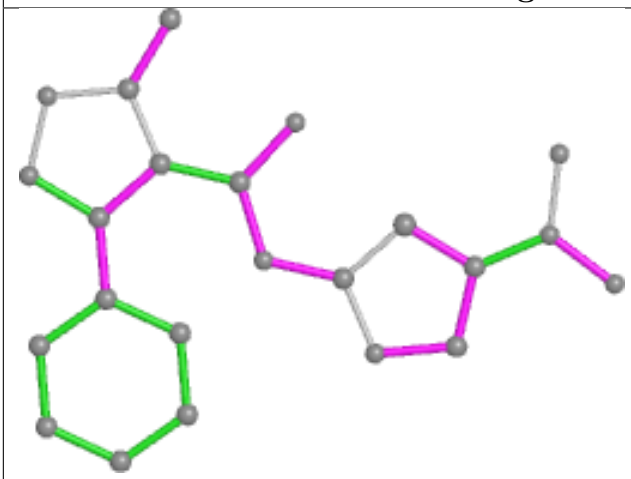


Rings

Ligand EHL E 2302



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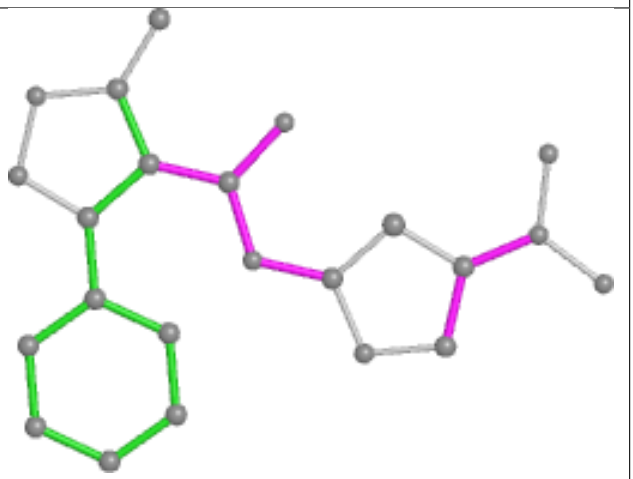

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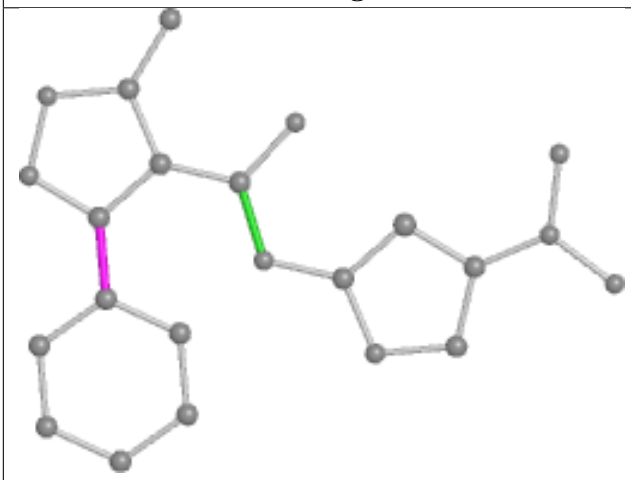

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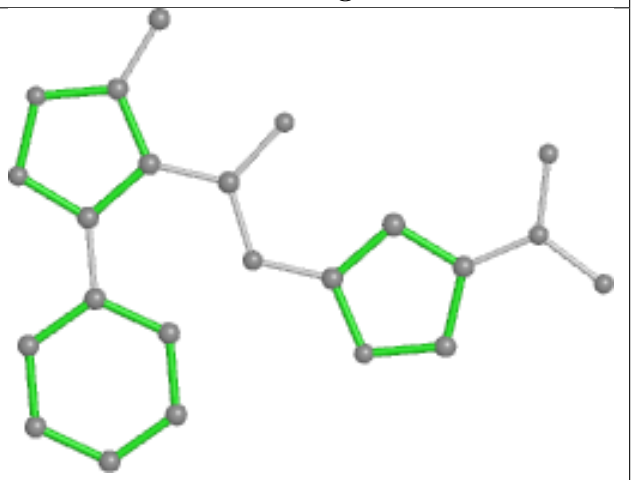
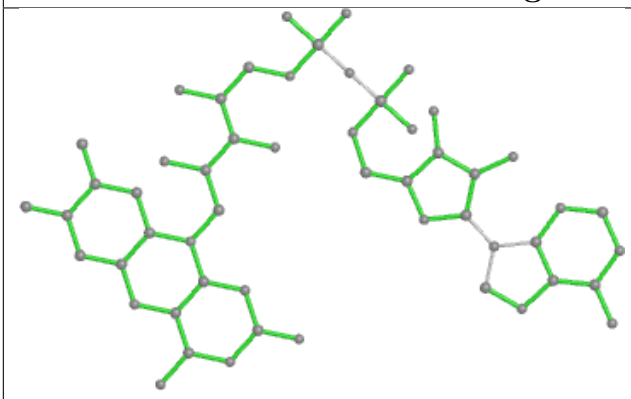


Rings

Ligand FAD D 302



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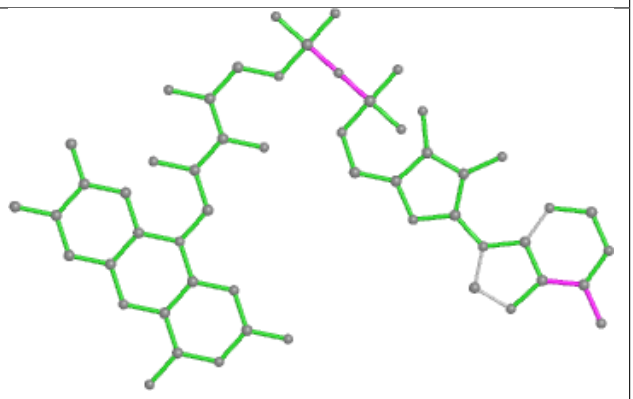
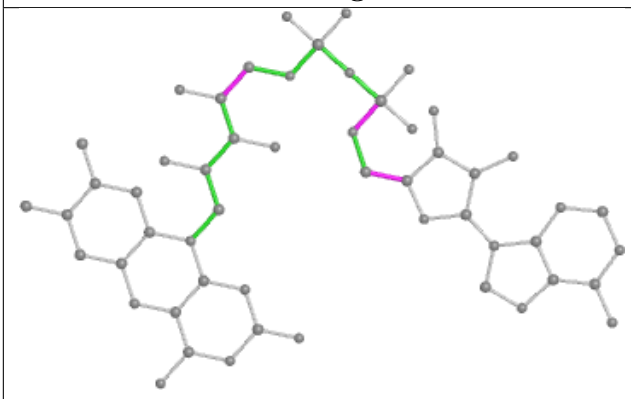


Bond angles



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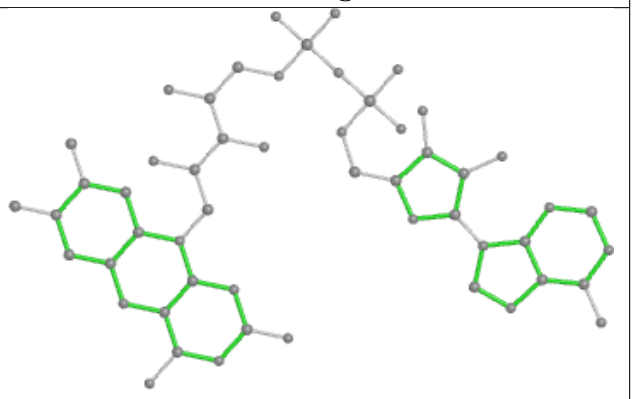
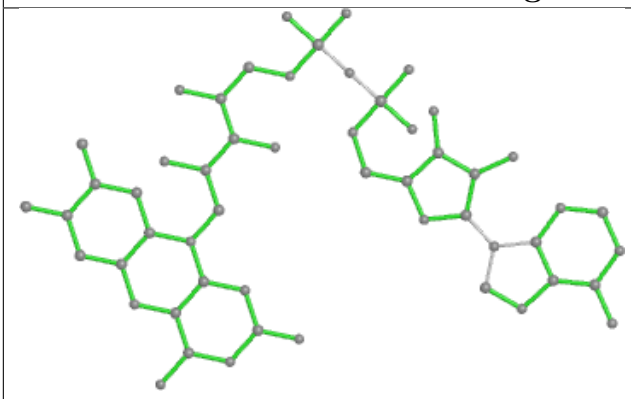


Rings

Ligand FAD H 302



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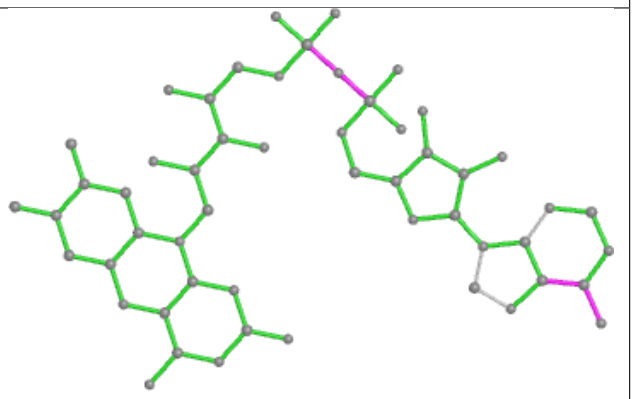

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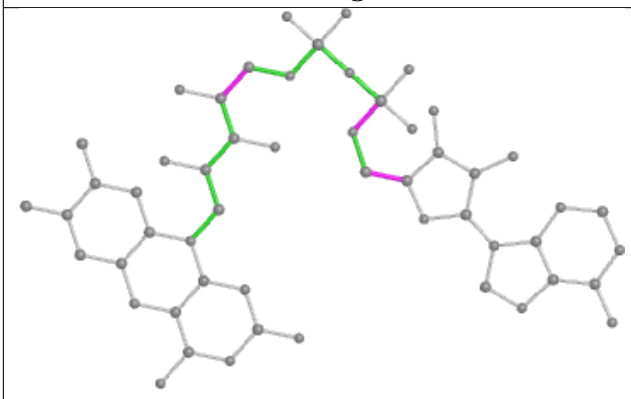
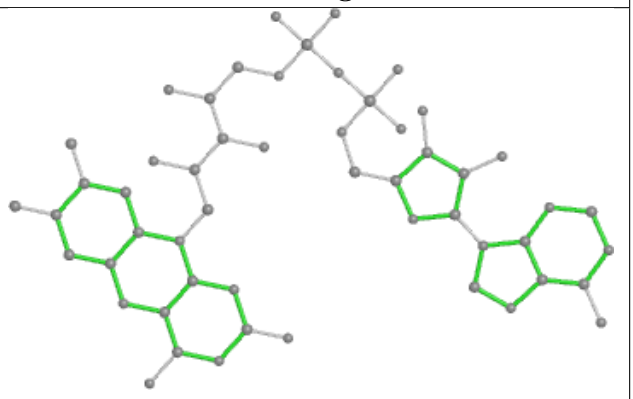
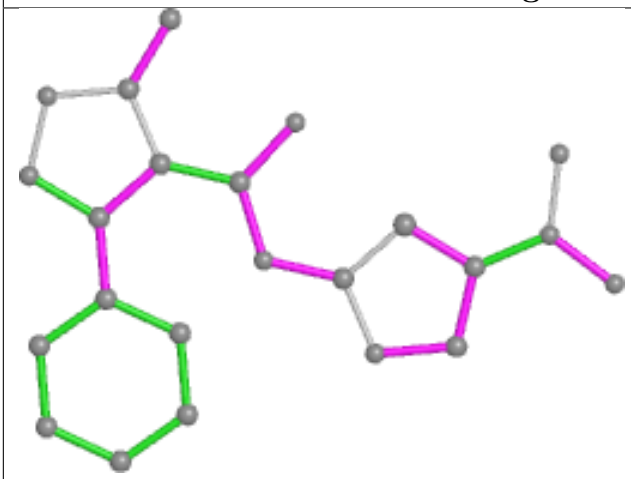


Torsions

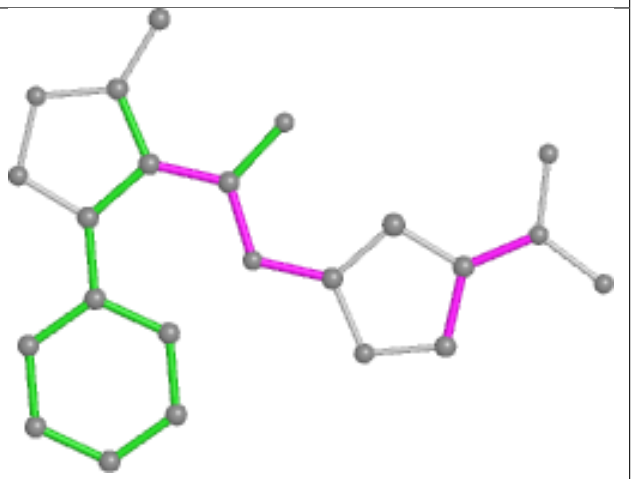


Rings

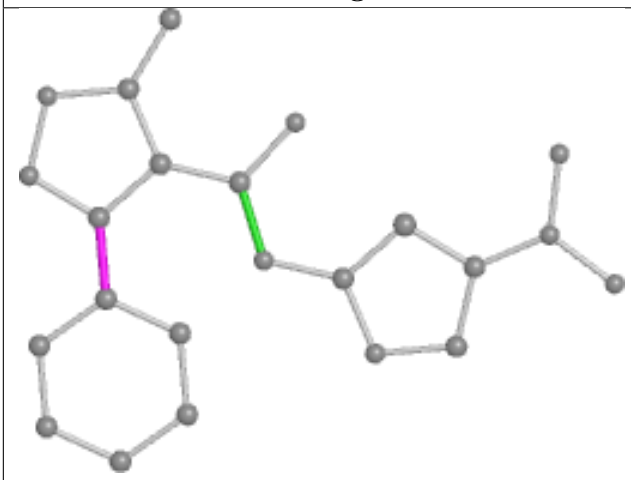
Ligand EHL I 2302



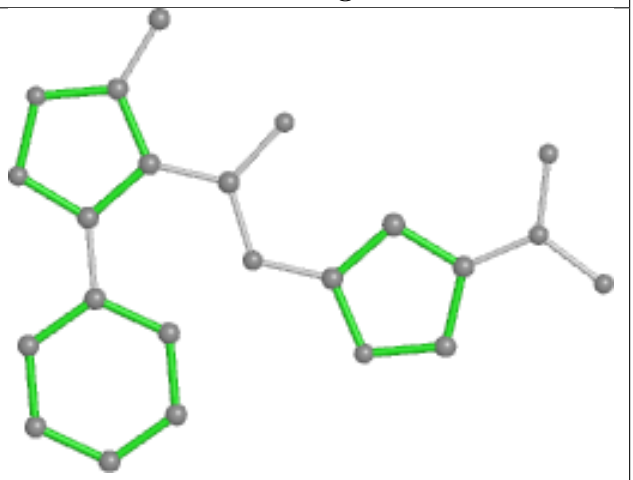
Bond lengths



Bond angles

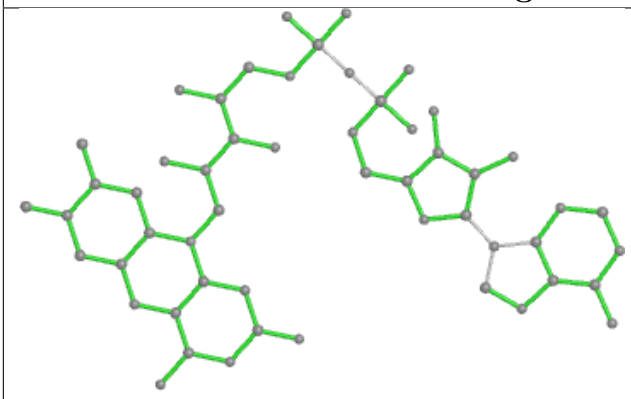


Torsions

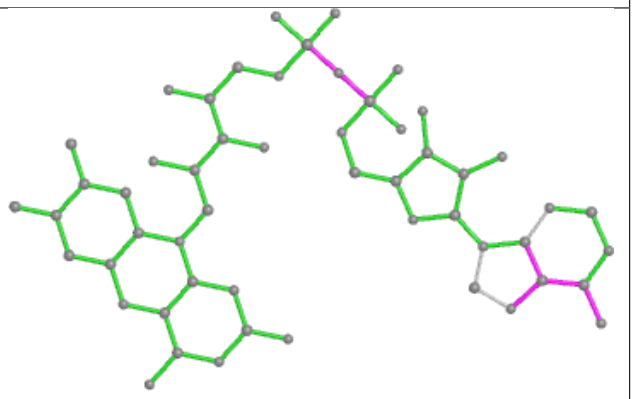


Rings

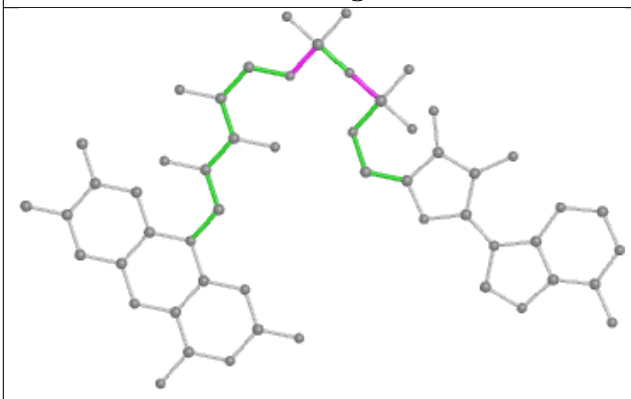
Ligand FAD A 2301



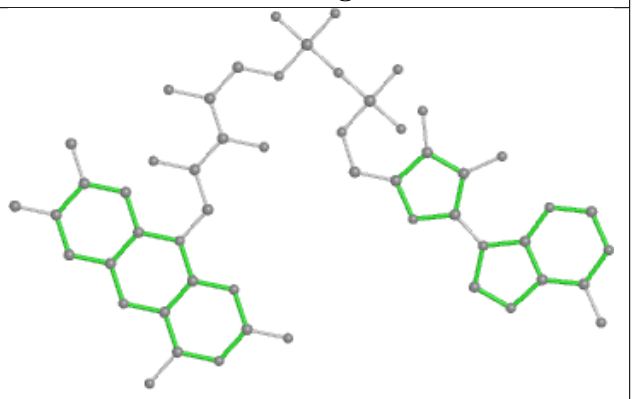
Bond lengths



Bond angles

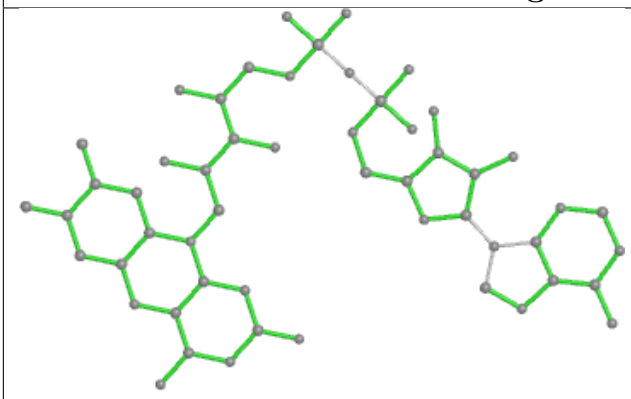


Torsions

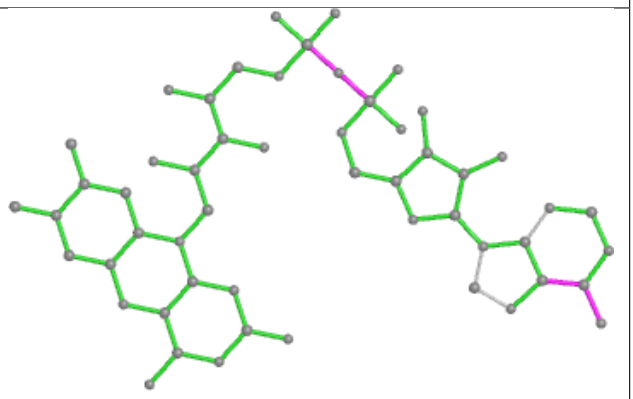


Rings

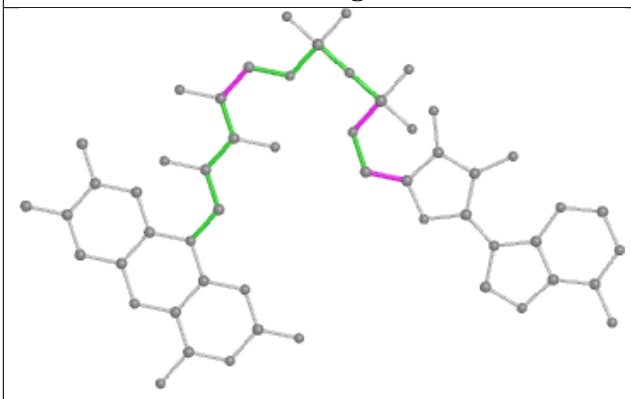
Ligand FAD L 302



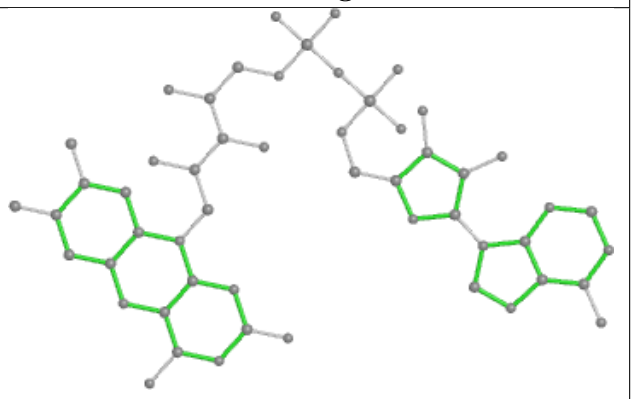
Bond lengths



Bond angles

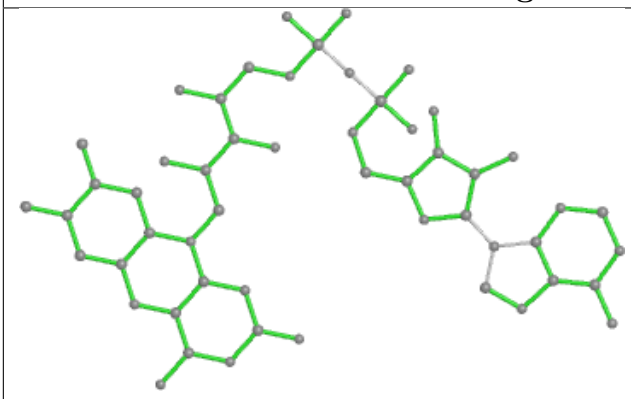


Torsions

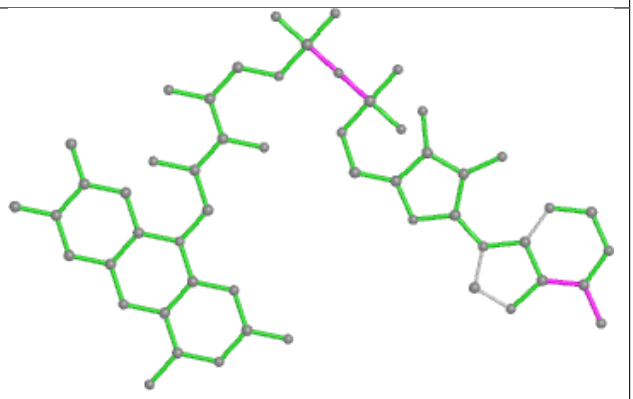


Rings

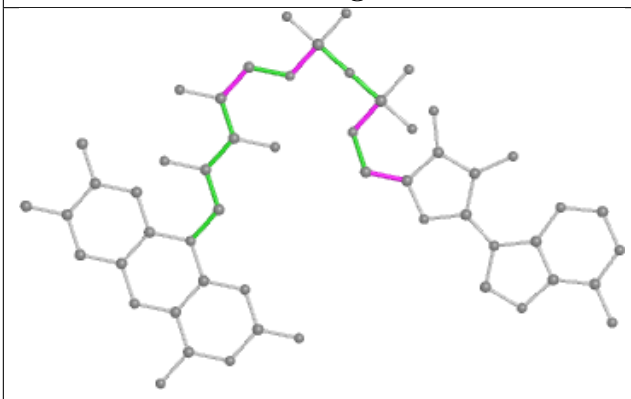
Ligand FAD B 2301



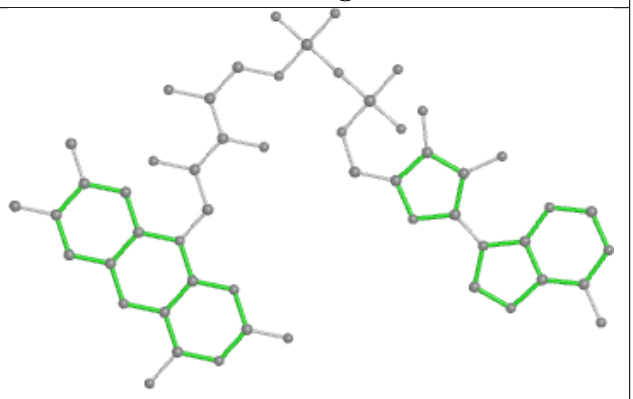
Bond lengths



Bond angles

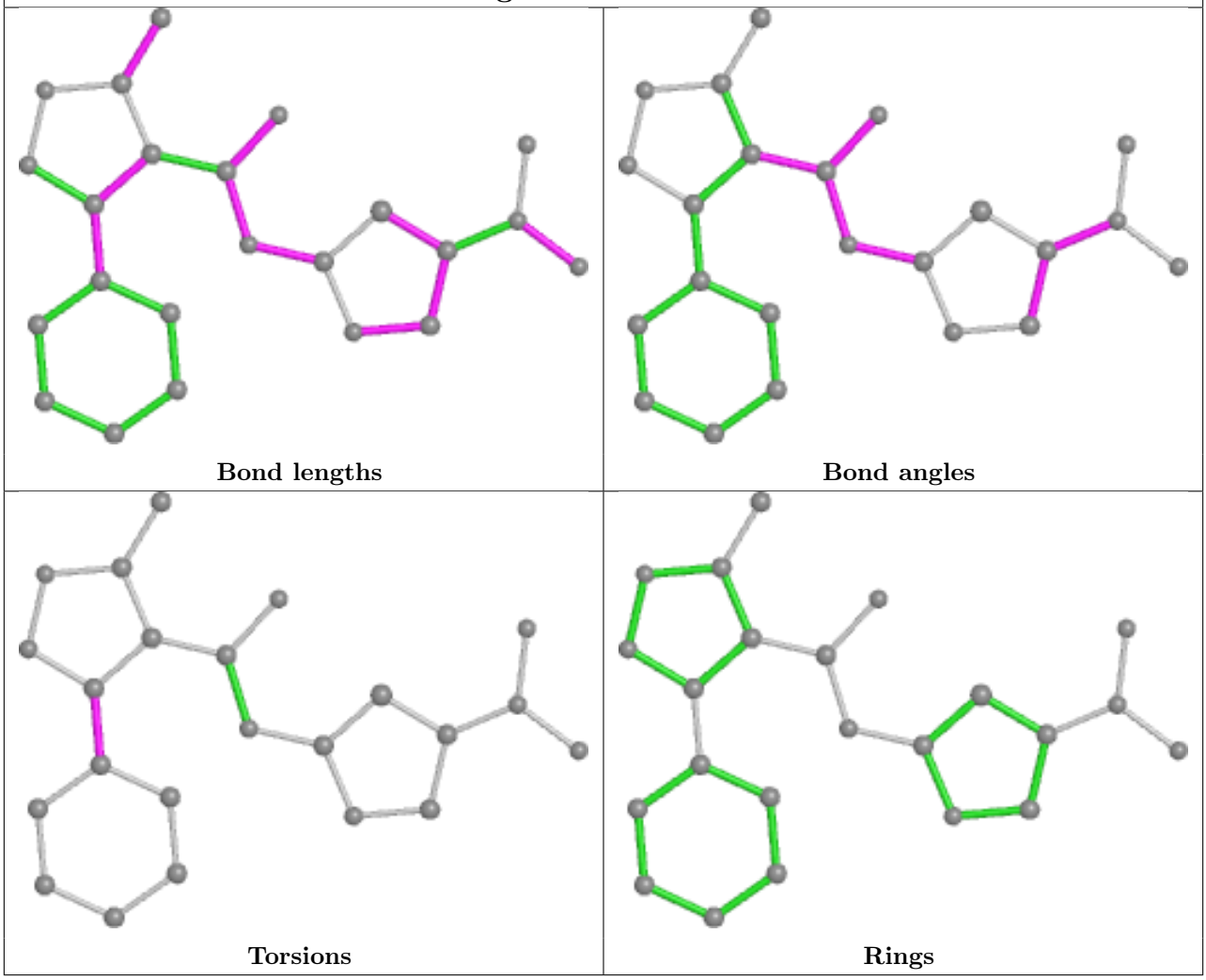


Torsions



Rings

Ligand EHL L 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	272/273 (99%)	-0.24	2 (0%)	87	89	21, 32, 57, 68	0
1	B	271/273 (99%)	0.17	12 (4%)	34	37	31, 47, 69, 81	0
1	C	271/273 (99%)	-0.15	9 (3%)	46	50	22, 39, 65, 76	0
1	D	272/273 (99%)	-0.14	8 (2%)	51	55	21, 31, 55, 69	0
1	E	271/273 (99%)	0.07	6 (2%)	62	65	22, 41, 60, 78	0
1	F	271/273 (99%)	-0.10	7 (2%)	56	59	32, 46, 67, 81	0
1	G	270/273 (98%)	0.10	11 (4%)	37	40	28, 45, 67, 85	0
1	H	270/273 (98%)	0.03	10 (3%)	41	45	30, 46, 68, 82	0
1	I	270/273 (98%)	0.10	9 (3%)	46	50	32, 48, 71, 87	0
1	J	270/273 (98%)	-0.07	9 (3%)	46	50	30, 46, 68, 84	0
1	K	271/273 (99%)	-0.02	15 (5%)	25	26	32, 48, 73, 86	0
1	L	271/273 (99%)	0.35	20 (7%)	14	15	34, 51, 72, 85	0
All	All	3250/3276 (99%)	0.01	118 (3%)	42	46	21, 44, 68, 87	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	128	TYR	8.2
1	G	128	TYR	7.1
1	J	232	PHE	6.5
1	H	128	TYR	6.4
1	G	58	LYS	4.9
1	F	128	TYR	4.6
1	B	232	PHE	4.6
1	I	128	TYR	4.5
1	K	128	TYR	4.5
1	K	232	PHE	4.5
1	L	232	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	128	TYR	4.3
1	J	198	ASP	4.3
1	K	62	PRO	4.2
1	I	248	ASN	3.9
1	E	128	TYR	3.9
1	G	240	LYS	3.8
1	B	233	GLN	3.8
1	F	2	GLY	3.8
1	J	64	ASN	3.7
1	L	199	ALA	3.6
1	I	232	PHE	3.5
1	H	64	ASN	3.5
1	H	232	PHE	3.5
1	E	232	PHE	3.4
1	I	233	GLN	3.4
1	D	273	LYS	3.4
1	C	232	PHE	3.3
1	C	64	ASN	3.2
1	B	58	LYS	3.2
1	H	198	ASP	3.1
1	J	58	LYS	3.1
1	L	14	ARG	3.1
1	L	247	LYS	3.1
1	H	63	ALA	3.1
1	K	63	ALA	3.1
1	H	60	LYS	3.0
1	C	247	LYS	3.0
1	F	3	ARG	3.0
1	K	61	ASP	2.9
1	I	240	LYS	2.9
1	B	3	ARG	2.8
1	D	58	LYS	2.8
1	C	63	ALA	2.8
1	F	64	ASN	2.8
1	D	128	TYR	2.8
1	K	233	GLN	2.8
1	K	64	ASN	2.8
1	I	247	LYS	2.7
1	K	201	ILE	2.7
1	B	2	GLY	2.7
1	G	233	GLN	2.7
1	E	3	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	196	PRO	2.6
1	B	128	TYR	2.6
1	G	63	ALA	2.6
1	L	2	GLY	2.5
1	L	144	LEU	2.5
1	H	31	LYS	2.5
1	D	62	PRO	2.5
1	D	64	ASN	2.5
1	K	240	LYS	2.5
1	I	234	ALA	2.5
1	G	62	PRO	2.5
1	K	59	LEU	2.4
1	L	202	GLN	2.4
1	G	31	LYS	2.4
1	G	247	LYS	2.4
1	D	171	ILE	2.4
1	J	128	TYR	2.4
1	E	60	LYS	2.4
1	B	240	LYS	2.4
1	L	61	ASP	2.4
1	L	64	ASN	2.3
1	L	8	VAL	2.3
1	I	14	ARG	2.3
1	L	244	ASP	2.3
1	J	201	ILE	2.3
1	L	171	ILE	2.3
1	B	201	ILE	2.3
1	A	273	LYS	2.3
1	K	198	ASP	2.3
1	C	240	LYS	2.3
1	J	202	GLN	2.2
1	E	241	GLU	2.2
1	F	198	ASP	2.2
1	E	171	ILE	2.2
1	J	234	ALA	2.2
1	A	2	GLY	2.2
1	G	14	ARG	2.2
1	H	14	ARG	2.2
1	L	99	PHE	2.2
1	F	22	LYS	2.1
1	K	60	LYS	2.1
1	H	62	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	4	ARG	2.1
1	B	202	GLN	2.1
1	G	61	ASP	2.1
1	L	30	LYS	2.1
1	B	242	VAL	2.1
1	L	26	ALA	2.1
1	D	232	PHE	2.1
1	B	241	GLU	2.1
1	G	241	GLU	2.1
1	C	60	LYS	2.1
1	H	59	LEU	2.1
1	L	241	GLU	2.1
1	D	234	ALA	2.1
1	K	199	ALA	2.1
1	J	79	HIS	2.1
1	L	175	ILE	2.1
1	K	205	GLU	2.0
1	L	240	LYS	2.0
1	C	244	ASP	2.0
1	F	199	ALA	2.0
1	L	3	ARG	2.0
1	B	89	LYS	2.0
1	C	62	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.