



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 10:48 PM EDT

PDB ID : 6GND
Title : Crystal structure of the complex of a Ferredoxin-Flavin Thioredoxin Reductase and a Thioredoxin from *Clostridium acetobutylicum* at 2.9 Å resolution
Authors : Buey, R.M.; Fernandez-Justel, D.; Balsera, M.
Deposited on : 2018-05-30
Resolution : 2.89 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	:	2.37.1
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)	:	2.37.1

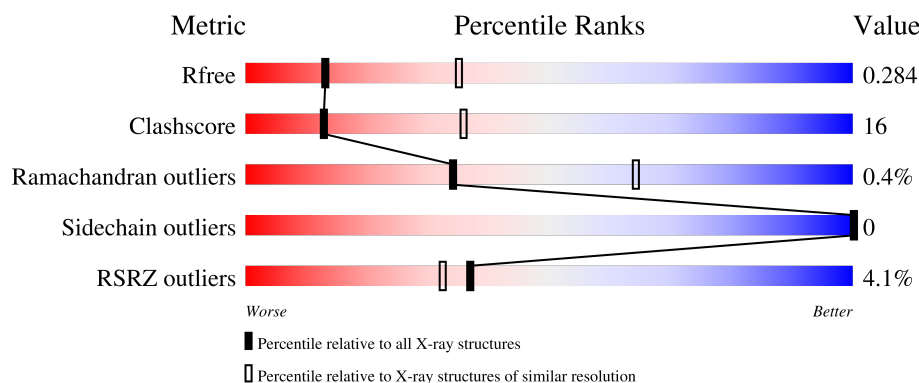
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	288	<div> <div>3%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	C	288	<div> <div>2%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
1	E	288	<div> <div>5%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>
1	G	288	<div> <div>5%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
2	B	108	<div> <div>4%</div> <div>64%</div> <div>22%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	108	 6% 66% 22% 12%
2	F	108	 4% 71% 12% 17%
2	H	108	 5% 64% 12% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20212 atoms, of which 9552 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 Thioredoxin reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	279	Total	C	H	N	O	S	0	0	0
			3974	1310	1940	327	387	10			
1	C	278	Total	C	H	N	O	S	0	0	0
			4054	1319	1993	338	394	10			
1	E	278	Total	C	H	N	O	S	0	1	0
			3733	1256	1778	327	364	8			
1	G	280	Total	C	H	N	O	S	0	0	0
			3681	1233	1744	329	364	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q97EM8
A	-1	SER	-	expression tag	UNP Q97EM8
A	0	HIS	-	expression tag	UNP Q97EM8
A	131	SER	CYS	engineered mutation	UNP Q97EM8
C	-2	GLY	-	expression tag	UNP Q97EM8
C	-1	SER	-	expression tag	UNP Q97EM8
C	0	HIS	-	expression tag	UNP Q97EM8
C	131	SER	CYS	engineered mutation	UNP Q97EM8
E	-2	GLY	-	expression tag	UNP Q97EM8
E	-1	SER	-	expression tag	UNP Q97EM8
E	0	HIS	-	expression tag	UNP Q97EM8
E	131	SER	CYS	engineered mutation	UNP Q97EM8
G	-2	GLY	-	expression tag	UNP Q97EM8
G	-1	SER	-	expression tag	UNP Q97EM8
G	0	HIS	-	expression tag	UNP Q97EM8
G	131	SER	CYS	engineered mutation	UNP Q97EM8

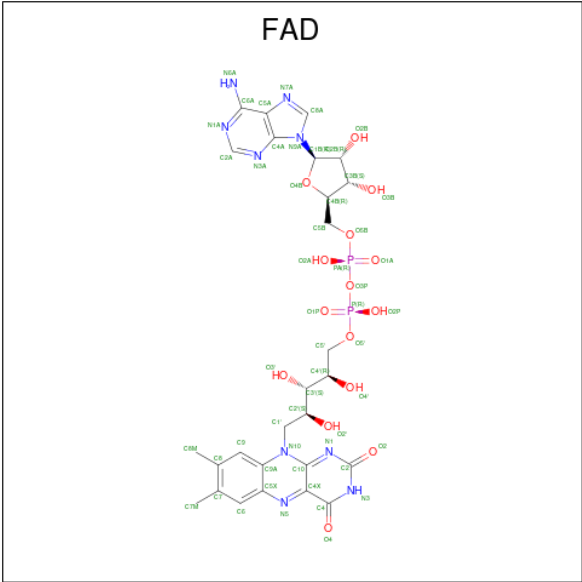
- Molecule 2 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	93	Total	C	H	N	O	S	0	0	0
			1166	404	536	103	120	3			
2	D	95	Total	C	H	N	O	S	0	0	0
			1189	413	550	105	119	2			
2	F	90	Total	C	H	N	O	S	0	0	0
			1028	368	448	96	113	3			
2	H	82	Total	C	H	N	O	S	0	0	0
			964	340	427	89	106	2			

There are 16 discrepancies between the modelled and reference sequences:

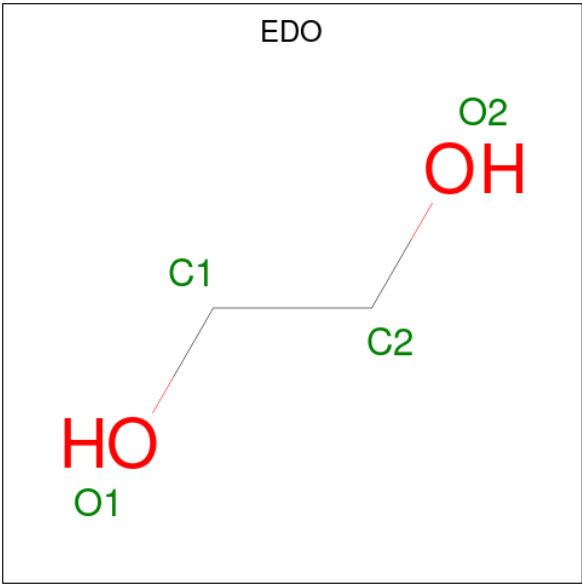
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q97EM7
B	-1	SER	-	expression tag	UNP Q97EM7
B	0	HIS	-	expression tag	UNP Q97EM7
B	33	SER	CYS	engineered mutation	UNP Q97EM7
D	-2	GLY	-	expression tag	UNP Q97EM7
D	-1	SER	-	expression tag	UNP Q97EM7
D	0	HIS	-	expression tag	UNP Q97EM7
D	33	SER	CYS	engineered mutation	UNP Q97EM7
F	-2	GLY	-	expression tag	UNP Q97EM7
F	-1	SER	-	expression tag	UNP Q97EM7
F	0	HIS	-	expression tag	UNP Q97EM7
F	33	SER	CYS	engineered mutation	UNP Q97EM7
H	-2	GLY	-	expression tag	UNP Q97EM7
H	-1	SER	-	expression tag	UNP Q97EM7
H	0	HIS	-	expression tag	UNP Q97EM7
H	33	SER	CYS	engineered mutation	UNP Q97EM7

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
3	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
3	E	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
3	G	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C H O 10 2 6 2	0	0
4	G	1	Total C H O 10 2 6 2	0	0

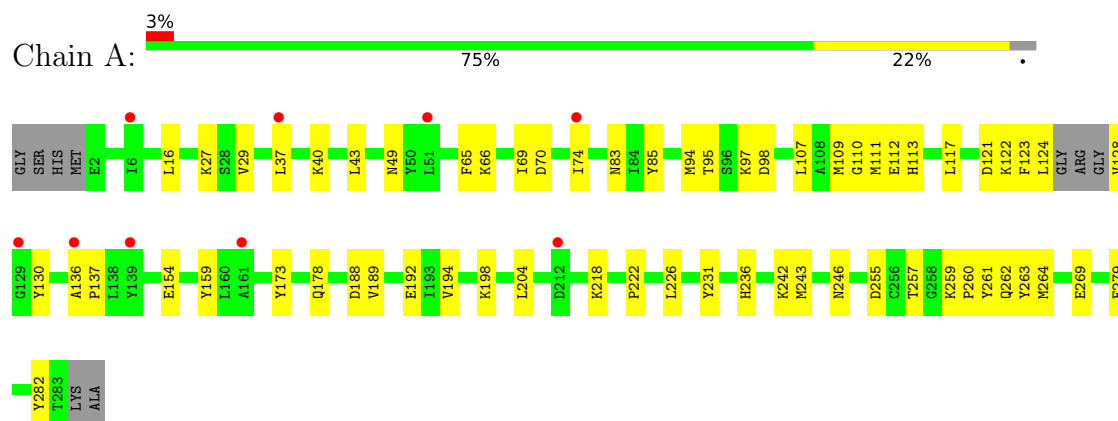
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	B	4	Total O 4 4	0	0
5	C	27	Total O 27 27	0	0
5	E	9	Total O 9 9	0	0
5	F	2	Total O 2 2	0	0
5	G	12	Total O 12 12	0	0
5	H	5	Total O 5 5	0	0

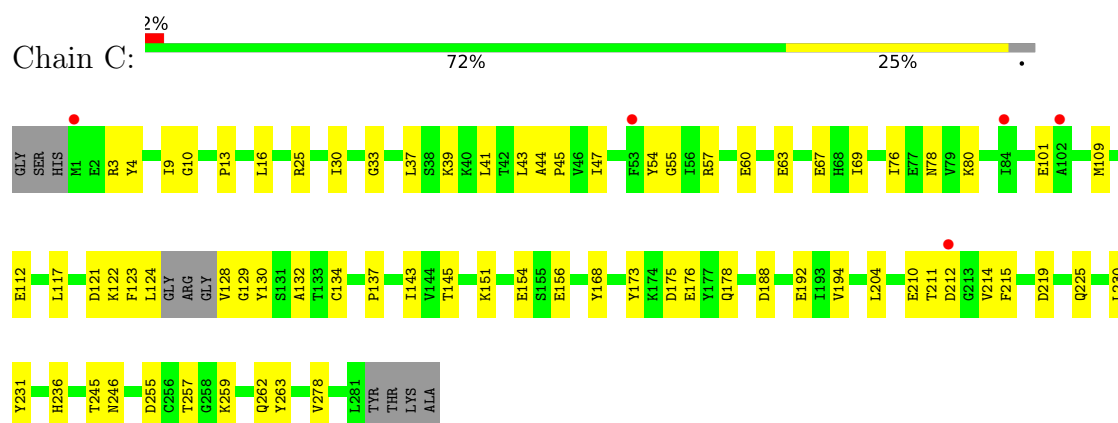
3 Residue-property plots [i](#)

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.

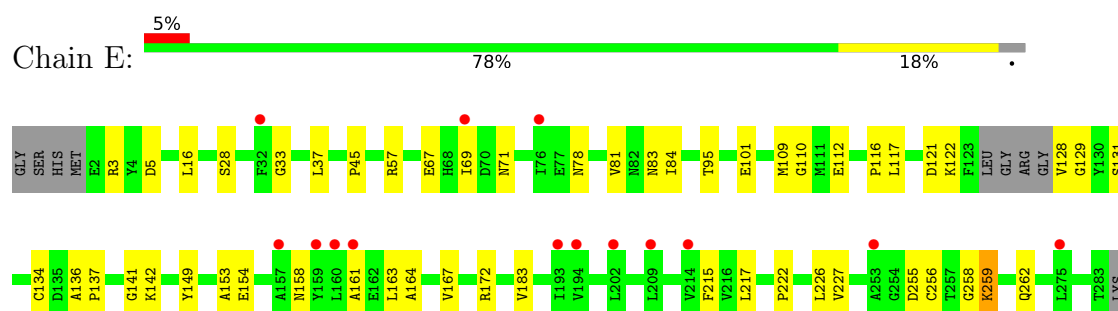
• Molecule 1: Thioredoxin reductase



• Molecule 1: Thioredoxin reductase




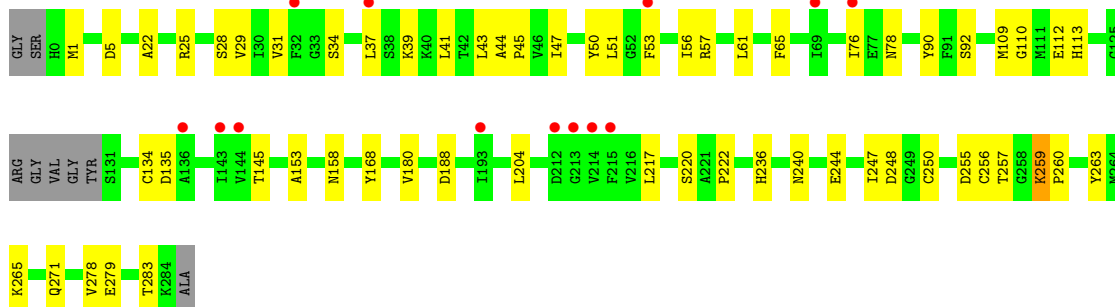
• Molecule 1: Thioredoxin reductase



ALA

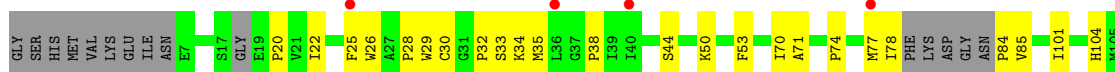
• Molecule 1: Thioredoxin reductase

Chain G:  5% 77% 20%



• Molecule 2: Thioredoxin

Chain B:  4% 64% 22% 14%



• Molecule 2: Thioredoxin

Chain D:  6% 66% 22% 12%



M105

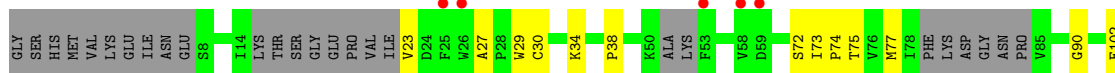
• Molecule 2: Thioredoxin

Chain F:  4% 71% 12% 17%



• Molecule 2: Thioredoxin

Chain H:  5% 64% 12% 24%



M105

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.23Å 174.35Å 114.30Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	86.74 – 2.89 87.17 – 2.89	Depositor EDS
% Data completeness (in resolution range)	63.3 (86.74-2.89) 63.3 (87.17-2.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.91Å)	Xtriage
Refinement program	PHENIX (dev_3026: ???)	Depositor
R, R_{free}	0.235 , 0.279 0.242 , 0.284	Depositor DCC
R_{free} test set	1314 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	90.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20212	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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, EDO

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	0.30	0/2069	0.51	0/2813
1	C	0.31	0/2095	0.51	0/2842
1	E	0.30	0/1991	0.48	0/2715
1	G	0.29	0/1968	0.49	0/2681
2	B	0.29	0/644	0.49	0/881
2	D	0.27	0/653	0.42	0/894
2	F	0.26	0/593	0.41	0/812
2	H	0.25	0/547	0.43	0/750
All	All	0.29	0/10560	0.48	0/14388

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2034	1940	1932	66	0
1	C	2061	1993	1993	85	0
1	E	1955	1778	1782	43	0
1	G	1937	1744	1743	53	0
2	B	630	536	533	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	639	550	545	40	0
2	F	580	448	447	9	0
2	H	537	427	424	15	0
3	A	53	31	31	4	0
3	C	53	31	31	12	0
3	E	53	31	31	10	0
3	G	53	31	31	4	0
4	C	4	6	6	0	0
4	G	4	6	6	0	0
5	A	8	0	0	0	0
5	B	4	0	0	0	0
5	C	27	0	0	0	0
5	E	9	0	0	0	0
5	F	2	0	0	0	0
5	G	12	0	0	2	0
5	H	5	0	0	0	0
All	All	10660	9552	9535	331	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 16.

All (331) 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:A:123:PHE:O	2:B:71:ALA:CB	1.68	1.39
1:A:123:PHE:O	2:B:71:ALA:HB1	1.14	1.30
1:G:134:CYS:SG	2:H:30:CYS:CB	2.19	1.29
2:B:22:ILE:HG12	2:B:78:ILE:CG2	1.62	1.28
1:G:134:CYS:SG	2:H:30:CYS:SG	1.25	1.17
2:D:47:LEU:O	2:D:49:GLY:HA2	1.44	1.14
2:B:25:PHE:CE2	2:B:77:MET:HE3	1.84	1.13
1:C:121:ASP:O	1:C:128:VAL:HG11	1.46	1.11
2:B:28:PRO:O	2:B:34:LYS:NZ	1.83	1.10
2:B:22:ILE:HG12	2:B:78:ILE:HG22	1.19	1.10
2:B:25:PHE:CE2	2:B:77:MET:CE	2.37	1.08
1:A:94:MET:CE	2:B:35:MET:HE3	1.84	1.07
2:B:22:ILE:CG1	2:B:78:ILE:HG22	1.84	1.07
1:C:121:ASP:O	1:C:128:VAL:CG1	2.03	1.06
1:E:255:ASP:OD1	3:E:300:FAD:C5'	2.06	1.04
1:A:121:ASP:O	1:A:128:VAL:HG23	1.58	1.03
1:A:124:LEU:O	1:A:128:VAL:N	1.95	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ASP:OD1	3:E:300:FAD:O2P	1.80	0.98
1:A:94:MET:CE	2:B:35:MET:CE	2.43	0.97
1:G:135:ASP:OD1	2:H:73:ILE:N	1.98	0.96
1:C:132:ALA:HB3	1:C:156:GLU:OE1	1.66	0.95
1:E:255:ASP:OD1	3:E:300:FAD:H5'1	1.67	0.94
2:B:25:PHE:HE2	2:B:77:MET:HE3	1.18	0.93
1:C:80:LYS:NZ	1:C:219:ASP:O	2.01	0.93
1:C:151:LYS:NZ	1:C:178:GLN:OE1	2.00	0.93
1:E:255:ASP:OD1	3:E:300:FAD:P	2.27	0.92
1:G:135:ASP:OD2	2:H:72:SER:HA	1.69	0.91
1:A:40:LYS:HZ1	1:A:111:MET:HE1	1.35	0.91
1:A:124:LEU:C	1:A:128:VAL:N	2.26	0.90
1:C:134:CYS:O	2:D:73:ILE:HD12	1.71	0.88
2:B:25:PHE:HE2	2:B:77:MET:CE	1.80	0.88
1:A:113:HIS:HE1	1:A:218:LYS:HD3	1.37	0.88
1:A:95:THR:OG1	1:A:98:ASP:O	1.90	0.87
1:A:97:LYS:O	1:A:98:ASP:OD1	1.91	0.87
1:A:94:MET:HE3	2:B:35:MET:CE	2.04	0.87
1:E:129:GLY:O	1:E:215:PHE:CD1	2.28	0.87
2:B:26:TRP:HB2	2:B:33:SER:HB2	1.59	0.85
1:G:134:CYS:SG	2:H:30:CYS:HB2	2.15	0.84
1:A:40:LYS:NZ	1:A:111:MET:HE1	1.92	0.84
1:C:41:LEU:HD21	1:C:263:TYR:CE1	2.13	0.83
1:C:41:LEU:CD2	1:C:263:TYR:CE1	2.61	0.83
1:E:112:GLU:OE2	1:E:112:GLU:N	2.10	0.82
1:G:39:LYS:O	1:G:43:LEU:HG	1.79	0.82
1:C:47:ILE:HD13	1:C:263:TYR:CE2	2.15	0.81
1:E:109:MET:O	1:E:256:CYS:HB3	1.80	0.81
1:C:117:LEU:CD1	1:C:192:GLU:HG3	2.10	0.81
2:D:29:TRP:HE1	2:D:73:ILE:CD1	1.94	0.81
1:A:40:LYS:NZ	1:A:111:MET:CE	2.44	0.80
2:D:29:TRP:NE1	2:D:73:ILE:CD1	2.45	0.80
1:G:45:PRO:O	1:G:57:ARG:HD3	1.81	0.80
2:B:26:TRP:CB	2:B:33:SER:HB2	2.11	0.79
1:C:188:ASP:HB3	1:C:204:LEU:HD23	1.63	0.79
2:B:25:PHE:CZ	2:B:77:MET:CE	2.64	0.79
1:A:94:MET:HE1	2:B:35:MET:HE3	1.64	0.79
1:C:134:CYS:HB3	2:D:30:CYS:SG	2.22	0.79
1:C:134:CYS:HG	2:D:30:CYS:HG	1.18	0.78
2:B:44:SER:HA	2:B:53:PHE:CE2	2.18	0.78
2:D:29:TRP:HE1	2:D:73:ILE:HD12	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HZ1	1:A:111:MET:CE	1.97	0.76
1:A:123:PHE:O	2:B:71:ALA:HB3	1.79	0.76
2:B:22:ILE:HG12	2:B:78:ILE:HG21	1.66	0.76
2:B:85:VAL:CB	2:B:104:HIS:NE2	2.48	0.76
1:G:44:ALA:HA	3:G:301:FAD:HM72	1.66	0.76
1:A:112:GLU:HG3	1:A:222:PRO:HA	1.69	0.75
2:B:22:ILE:HD11	2:B:101:ILE:HD11	1.69	0.74
2:B:25:PHE:CZ	2:B:77:MET:HE3	2.23	0.72
1:C:134:CYS:CB	2:D:30:CYS:SG	2.76	0.72
2:D:47:LEU:C	2:D:49:GLY:HA2	2.10	0.72
1:C:117:LEU:HD13	1:C:192:GLU:HG3	1.71	0.71
1:C:130:TYR:CE2	1:C:225:GLN:OE1	2.44	0.71
1:E:121:ASP:O	1:E:128:VAL:CB	2.38	0.71
2:B:34:LYS:O	2:B:38:PRO:CD	2.39	0.71
1:G:158:ASN:OD1	1:G:180:VAL:HG13	1.91	0.70
2:B:22:ILE:CD1	2:B:101:ILE:HD11	2.21	0.70
1:C:255:ASP:OD2	3:C:301:FAD:H5'1	1.91	0.70
1:A:117:LEU:HD22	1:A:192:GLU:HG3	1.73	0.70
2:D:50:LYS:HD2	2:D:50:LYS:O	1.91	0.70
2:D:47:LEU:O	2:D:49:GLY:CA	2.31	0.70
1:A:113:HIS:CE1	1:A:218:LYS:HD3	2.25	0.70
1:E:255:ASP:OD1	3:E:300:FAD:H5'2	1.92	0.69
2:B:34:LYS:O	2:B:38:PRO:HD2	1.91	0.69
1:A:66:LYS:HE3	1:A:70:ASP:OD2	1.93	0.69
1:C:41:LEU:HD23	1:C:263:TYR:CE1	2.27	0.69
3:C:301:FAD:N1	3:C:301:FAD:H2'	2.07	0.69
1:E:255:ASP:CG	3:E:300:FAD:H5'1	2.13	0.69
1:G:37:LEU:O	3:G:301:FAD:O3B	2.11	0.69
1:G:248:ASP:O	5:G:401:HOH:O	2.11	0.69
1:E:129:GLY:O	1:E:215:PHE:HD1	1.74	0.68
1:E:16:LEU:HD22	1:E:69:ILE:HG21	1.75	0.68
2:D:29:TRP:CZ2	2:D:73:ILE:HD11	2.29	0.68
2:B:22:ILE:CG1	2:B:78:ILE:CG2	2.51	0.67
1:C:124:LEU:O	1:C:128:VAL:N	2.27	0.67
1:C:124:LEU:C	1:C:128:VAL:HG12	2.14	0.67
2:H:72:SER:O	2:H:75:THR:OG1	2.11	0.67
1:C:121:ASP:O	1:C:128:VAL:HG12	1.91	0.67
1:C:117:LEU:CD1	1:C:192:GLU:CG	2.72	0.67
1:C:175:ASP:OD1	1:C:176:GLU:N	2.28	0.66
1:E:110:GLY:HA2	1:E:255:ASP:HB2	1.78	0.66
1:C:121:ASP:C	1:C:128:VAL:HG11	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:CYS:CB	2:D:30:CYS:HG	2.10	0.65
2:D:39:ILE:CD1	2:D:91:PHE:CZ	2.79	0.64
1:C:117:LEU:HD12	1:C:192:GLU:HG3	1.76	0.64
1:G:112:GLU:HG3	1:G:222:PRO:HB3	1.79	0.64
1:C:117:LEU:HD12	1:C:192:GLU:CG	2.28	0.64
1:G:113:HIS:HE1	1:G:220:SER:CB	2.11	0.64
1:G:25:ARG:HD2	1:G:278:VAL:HG11	1.79	0.64
1:G:47:ILE:HD13	1:G:263:TYR:CE2	2.33	0.64
1:G:135:ASP:CG	2:H:73:ILE:H	2.00	0.63
1:C:122:LYS:O	1:C:128:VAL:HG13	1.98	0.63
1:A:43:LEU:O	1:A:43:LEU:HD23	1.99	0.63
2:H:102:GLU:OE1	2:H:102:GLU:HA	1.99	0.63
2:B:22:ILE:HD12	2:B:53:PHE:CE1	2.35	0.62
2:B:85:VAL:CB	2:B:104:HIS:CD2	2.83	0.62
2:D:39:ILE:HD11	2:D:91:PHE:CZ	2.33	0.62
1:G:1:MET:O	1:G:1:MET:HG3	1.99	0.62
1:A:40:LYS:HZ2	1:A:111:MET:HE2	1.65	0.62
1:C:39:LYS:O	1:C:43:LEU:HG	2.00	0.61
1:C:124:LEU:C	1:C:128:VAL:N	2.53	0.61
1:C:263:TYR:CE1	3:C:301:FAD:O2'	2.53	0.61
1:A:236:HIS:ND1	1:A:257:THR:O	2.33	0.61
1:C:123:PHE:O	2:D:71:ALA:CB	2.49	0.61
1:G:47:ILE:HD12	1:G:61:LEU:HD22	1.82	0.61
1:A:124:LEU:CB	1:A:198:LYS:HB2	2.30	0.60
1:C:117:LEU:HD12	1:C:192:GLU:CB	2.32	0.60
1:A:40:LYS:HZ2	1:A:111:MET:CE	2.14	0.60
2:B:25:PHE:CE2	2:B:77:MET:HE2	2.35	0.60
1:C:143:ILE:N	1:C:212:ASP:OD2	2.33	0.60
1:E:84:ILE:HB	1:E:227:VAL:HG22	1.83	0.60
1:A:112:GLU:OE1	1:A:112:GLU:N	2.35	0.59
2:F:85:VAL:CB	2:F:104:HIS:ND1	2.65	0.59
1:C:128:VAL:HG13	1:C:128:VAL:O	2.02	0.59
2:B:25:PHE:CZ	2:B:77:MET:HE1	2.37	0.59
2:D:39:ILE:HD12	2:D:91:PHE:CE2	2.38	0.59
1:E:33:GLY:O	1:E:78:ASN:HA	2.02	0.59
1:A:94:MET:CE	2:B:35:MET:HE2	2.31	0.59
1:G:236:HIS:HB2	1:G:257:THR:O	2.04	0.58
1:C:151:LYS:NZ	1:C:154:GLU:OE1	2.29	0.58
1:C:192:GLU:HG2	1:C:194:VAL:HG13	1.85	0.57
2:B:44:SER:HA	2:B:53:PHE:HE2	1.65	0.57
2:B:44:SER:HA	2:B:53:PHE:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ALA:HB2	3:C:301:FAD:C6	2.34	0.57
1:A:94:MET:HE2	2:B:35:MET:CE	2.34	0.57
1:A:178:GLN:HB3	1:C:178:GLN:HB3	1.86	0.57
2:D:39:ILE:CD1	2:D:91:PHE:CE2	2.88	0.57
1:E:83:ASN:HA	1:E:226:LEU:HD12	1.86	0.57
1:A:113:HIS:HE1	1:A:218:LYS:CD	2.15	0.56
2:B:20:PRO:HD2	2:B:50:LYS:O	2.05	0.56
1:G:188:ASP:CB	1:G:204:LEU:HD23	2.36	0.56
1:G:22:ALA:HB3	1:G:29:VAL:HG21	1.88	0.56
3:A:300:FAD:O2'	3:A:300:FAD:O4'	2.11	0.56
1:C:37:LEU:O	3:C:301:FAD:O3B	2.16	0.56
1:G:113:HIS:CE1	1:G:220:SER:CB	2.88	0.56
1:A:121:ASP:O	1:A:128:VAL:CG2	2.46	0.55
1:C:9:ILE:CG2	1:C:109:MET:HE3	2.36	0.55
1:E:153:ALA:HA	1:E:217:LEU:HD12	1.88	0.55
1:C:57:ARG:HB2	1:C:60:GLU:HG3	1.87	0.55
1:C:145:THR:HG23	1:C:168:TYR:HB2	1.89	0.55
1:E:45:PRO:O	1:E:57:ARG:HA	2.07	0.55
2:F:34:LYS:O	2:F:38:PRO:HD2	2.07	0.55
1:A:188:ASP:OD1	1:A:189:VAL:N	2.37	0.54
1:A:192:GLU:HG2	1:A:194:VAL:HG13	1.88	0.54
1:A:113:HIS:NE2	1:A:218:LYS:HB3	2.23	0.54
1:G:41:LEU:HD11	1:G:65:PHE:CE2	2.43	0.54
1:C:117:LEU:HD13	1:C:192:GLU:CG	2.35	0.54
1:G:260:PRO:O	1:G:265:LYS:HE2	2.08	0.54
1:A:40:LYS:NZ	1:A:111:MET:HE2	2.18	0.54
1:C:63:GLU:O	1:C:67:GLU:HG3	2.08	0.53
1:C:210:GLU:O	1:C:210:GLU:HG2	2.09	0.53
1:E:122:LYS:O	1:E:128:VAL:O	2.26	0.53
2:B:25:PHE:CE2	2:B:70:ILE:HD11	2.43	0.53
2:B:22:ILE:HG13	2:B:78:ILE:HG22	1.87	0.53
1:C:211:THR:HG21	1:C:214:VAL:HG22	1.89	0.53
1:C:123:PHE:O	2:D:71:ALA:HB3	2.09	0.53
2:D:29:TRP:NE1	2:D:73:ILE:HD12	2.17	0.53
1:G:5:ASP:OD1	1:G:28:SER:CB	2.57	0.52
1:G:135:ASP:OD1	2:H:73:ILE:CB	2.57	0.52
1:E:117:LEU:N	1:E:117:LEU:HD12	2.25	0.52
1:G:47:ILE:HD12	1:G:61:LEU:CD2	2.39	0.52
2:D:26:TRP:HB2	2:D:33:SER:HB2	1.90	0.52
1:E:3:ARG:HD2	1:E:101:GLU:HB3	1.92	0.52
2:B:34:LYS:O	2:B:38:PRO:HD3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD22	1:A:69:ILE:HG21	1.92	0.52
2:D:29:TRP:CE2	2:D:73:ILE:HD11	2.44	0.52
1:A:117:LEU:HD12	1:A:117:LEU:N	2.25	0.52
2:D:29:TRP:CE2	2:D:73:ILE:CD1	2.93	0.52
2:D:39:ILE:HD11	2:D:91:PHE:HZ	1.74	0.51
2:F:72:SER:OG	2:F:75:THR:OG1	2.29	0.51
2:D:26:TRP:CB	2:D:33:SER:HB2	2.41	0.51
1:C:137:PRO:HG2	2:D:29:TRP:CE2	2.46	0.51
1:C:231:TYR:N	1:C:246:ASN:OD1	2.31	0.51
1:C:117:LEU:HD12	1:C:192:GLU:HB2	1.93	0.50
1:G:135:ASP:CG	2:H:72:SER:HA	2.31	0.50
1:G:153:ALA:CB	1:G:217:LEU:HD12	2.41	0.50
1:A:94:MET:HE2	2:B:35:MET:HE2	1.93	0.50
1:E:137:PRO:HG2	2:F:29:TRP:CZ2	2.46	0.50
2:H:34:LYS:O	2:H:38:PRO:HD2	2.11	0.50
1:E:81:VAL:HA	1:E:95:THR:HG22	1.93	0.50
1:E:258:GLY:O	1:E:259:LYS:CB	2.59	0.50
1:C:25:ARG:HD2	1:C:278:VAL:HG11	1.92	0.50
1:G:41:LEU:HD11	1:G:65:PHE:HE2	1.77	0.50
1:A:136:ALA:CB	1:A:159:TYR:HE2	2.24	0.50
2:B:70:ILE:HD11	2:B:77:MET:CE	2.42	0.50
1:E:37:LEU:O	3:E:300:FAD:O3B	2.20	0.50
1:C:154:GLU:OE2	1:C:173:TYR:OH	2.22	0.49
1:E:129:GLY:O	1:E:215:PHE:HA	2.12	0.49
1:E:131:SER:CB	1:E:134:CYS:HB3	2.41	0.49
1:A:83:ASN:HA	1:A:226:LEU:HD12	1.94	0.49
2:D:27:ALA:HB3	2:D:73:ILE:HD13	1.94	0.49
1:A:110:GLY:HA2	1:A:255:ASP:HB2	1.93	0.49
1:C:123:PHE:O	2:D:71:ALA:HB1	2.12	0.49
2:D:29:TRP:HZ2	2:D:73:ILE:HD11	1.78	0.49
1:C:13:PRO:HD2	3:C:301:FAD:O1P	2.11	0.49
1:A:154:GLU:OE2	1:A:173:TYR:OH	2.25	0.48
1:E:142:LYS:O	1:E:164:ALA:HB1	2.13	0.48
1:C:262:GLN:HA	1:C:262:GLN:NE2	2.28	0.48
2:D:25:PHE:CD2	2:D:70:ILE:HD11	2.49	0.48
1:G:44:ALA:HB2	3:G:301:FAD:C6	2.43	0.48
1:G:112:GLU:HG3	1:G:222:PRO:CB	2.43	0.48
1:A:117:LEU:HD22	1:A:192:GLU:CG	2.40	0.48
1:G:260:PRO:O	1:G:265:LYS:CE	2.62	0.48
1:A:65:PHE:CD1	1:G:51:LEU:HG	2.49	0.48
1:C:57:ARG:HB2	1:C:60:GLU:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:GLY:O	1:C:215:PHE:HA	2.14	0.48
1:E:5:ASP:OD1	1:E:28:SER:CB	2.62	0.48
1:A:279:GLU:O	1:A:282:TYR:O	2.31	0.48
1:G:50:TYR:CD1	1:G:53:PHE:HD2	2.32	0.48
1:G:47:ILE:CD1	1:G:263:TYR:CE2	2.97	0.47
1:G:109:MET:O	1:G:256:CYS:HB3	2.15	0.47
2:D:23:VAL:HG13	2:D:56:VAL:HG23	1.96	0.47
1:G:135:ASP:OD2	2:H:72:SER:CA	2.51	0.47
1:A:154:GLU:HG3	1:A:173:TYR:OH	2.15	0.47
1:A:204:LEU:N	1:A:204:LEU:HD12	2.29	0.47
3:C:301:FAD:N1	3:C:301:FAD:C2'	2.73	0.47
2:F:36:LEU:O	2:F:40:ILE:N	2.40	0.47
1:G:56:ILE:HG23	1:G:56:ILE:O	2.14	0.47
1:A:231:TYR:N	1:A:246:ASN:OD1	2.34	0.47
1:A:260:PRO:HG3	5:G:405:HOH:O	2.14	0.47
2:B:70:ILE:HD11	2:B:77:MET:HE2	1.96	0.47
1:E:67:GLU:O	1:E:71:ASN:OD1	2.33	0.47
1:C:255:ASP:CG	3:C:301:FAD:H5'1	2.35	0.47
1:E:167:VAL:CG1	1:E:183:VAL:HG22	2.45	0.46
1:E:161:ALA:HA	1:E:167:VAL:HG21	1.96	0.46
1:A:69:ILE:HB	1:A:74:ILE:HB	1.98	0.46
1:A:262:GLN:NE2	1:A:262:GLN:HA	2.31	0.46
2:D:29:TRP:NE1	2:D:73:ILE:HD11	2.26	0.46
2:H:23:VAL:N	2:H:77:MET:O	2.48	0.46
1:G:31:VAL:HB	1:G:76:ILE:HD13	1.98	0.46
1:E:255:ASP:CG	3:E:300:FAD:C5'	2.77	0.46
2:F:78:ILE:O	2:F:85:VAL:N	2.49	0.46
1:G:34:SER:HA	1:G:78:ASN:OD1	2.16	0.46
1:C:33:GLY:O	1:C:78:ASN:HA	2.16	0.46
1:E:262:GLN:HA	1:E:262:GLN:NE2	2.31	0.46
1:A:107:LEU:HB3	1:A:109:MET:HE2	1.99	0.45
2:B:22:ILE:HD11	2:B:101:ILE:CD1	2.42	0.45
1:C:112:GLU:N	1:C:112:GLU:OE1	2.45	0.45
1:G:22:ALA:CB	1:G:29:VAL:HG21	2.45	0.45
1:A:263:TYR:CD2	3:A:300:FAD:C2	2.99	0.45
1:C:54:TYR:CD1	1:C:55:GLY:N	2.84	0.45
2:D:22:ILE:HG13	2:D:78:ILE:HG12	1.99	0.45
1:C:9:ILE:HG21	1:C:109:MET:CE	2.47	0.45
1:G:90:TYR:HE2	1:G:92:SER:HG	1.61	0.45
2:B:30:CYS:SG	2:B:32:PRO:HD2	2.57	0.45
1:C:16:LEU:HD22	1:C:69:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:ALA:HB2	1:E:183:VAL:HG23	1.97	0.45
2:D:43:LEU:HD21	2:D:94:LYS:CG	2.46	0.45
2:H:74:PRO:O	2:H:90:GLY:N	2.47	0.45
2:D:30:CYS:SG	2:D:32:PRO:HD2	2.57	0.45
2:B:28:PRO:O	2:B:34:LYS:CE	2.61	0.44
2:F:28:PRO:HA	2:F:34:LYS:HE3	1.98	0.44
1:A:243:MET:HE2	1:A:269:GLU:HB3	2.00	0.44
2:D:22:ILE:HB	2:D:53:PHE:CD2	2.52	0.44
1:E:149:TYR:CE2	1:E:172:ARG:HG3	2.52	0.44
1:C:137:PRO:HG2	2:D:29:TRP:CZ2	2.53	0.44
1:C:9:ILE:CG2	1:C:109:MET:CE	2.96	0.44
1:G:90:TYR:HE2	1:G:92:SER:OG	2.01	0.44
1:C:41:LEU:HD23	1:C:263:TYR:CZ	2.52	0.43
2:F:30:CYS:SG	2:F:32:PRO:HD2	2.58	0.43
2:F:85:VAL:CB	2:F:104:HIS:CE1	3.02	0.43
1:A:242:LYS:O	1:A:243:MET:HB2	2.18	0.43
2:B:44:SER:CA	2:B:53:PHE:CD2	3.02	0.43
1:C:134:CYS:O	2:D:73:ILE:CD1	2.55	0.43
1:G:145:THR:HG23	1:G:168:TYR:HB2	2.00	0.43
1:C:47:ILE:CD1	1:C:263:TYR:CE2	2.95	0.43
1:A:85:TYR:HE2	1:A:94:MET:HG3	1.84	0.43
1:A:43:LEU:HD22	3:A:300:FAD:HM72	2.01	0.43
1:G:247:ILE:HB	1:G:250:CYS:HB3	2.01	0.43
1:C:204:LEU:N	1:C:204:LEU:HD12	2.33	0.43
1:E:149:TYR:CZ	1:E:172:ARG:HG3	2.54	0.43
1:E:154:GLU:O	1:E:158:ASN:ND2	2.45	0.42
1:A:49:ASN:HD21	1:A:262:GLN:NE2	2.17	0.42
1:G:110:GLY:HA2	1:G:255:ASP:HB2	2.01	0.42
1:G:240:ASN:ND2	1:G:244:GLU:HB2	2.33	0.42
3:A:300:FAD:H9	3:A:300:FAD:H1'1	1.83	0.42
1:A:137:PRO:HG2	2:B:29:TRP:CZ2	2.54	0.42
2:B:44:SER:CA	2:B:53:PHE:CE2	2.97	0.42
1:C:236:HIS:HB2	1:C:257:THR:O	2.19	0.42
1:E:255:ASP:OD2	3:E:300:FAD:H5'1	2.20	0.42
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.88	0.42
2:D:25:PHE:CE2	2:D:70:ILE:HD11	2.55	0.42
1:A:27:LYS:O	1:A:29:VAL:HG23	2.20	0.42
1:A:107:LEU:HB3	1:A:109:MET:CE	2.49	0.42
1:C:4:TYR:CD2	1:C:30:ILE:HB	2.55	0.42
1:C:44:ALA:CB	3:C:301:FAD:C6	2.98	0.41
1:C:230:LEU:HD11	1:C:245:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ILE:HB	1:C:109:MET:HE3	2.02	0.41
1:C:10:GLY:HA2	3:C:301:FAD:H1B	2.00	0.41
1:C:122:LYS:C	1:C:128:VAL:HG13	2.41	0.41
3:C:301:FAD:H1'1	3:C:301:FAD:H9	1.83	0.41
1:E:136:ALA:HB3	1:E:137:PRO:HD3	2.02	0.41
1:G:47:ILE:HD13	1:G:263:TYR:CD2	2.55	0.41
1:G:259:LYS:CB	1:G:260:PRO:CD	2.98	0.41
1:E:141:GLY:N	1:E:163:LEU:O	2.36	0.41
1:C:3:ARG:HG2	1:C:101:GLU:OE2	2.20	0.41
1:C:37:LEU:CD2	1:C:76:ILE:HG13	2.51	0.41
1:C:262:GLN:HA	3:C:301:FAD:O2	2.21	0.41
1:G:113:HIS:CE1	1:G:220:SER:H	2.39	0.41
1:A:264:MET:HB2	1:G:271:GLN:OE1	2.20	0.41
1:C:4:TYR:HE2	1:C:30:ILE:HD12	1.84	0.41
1:C:45:PRO:O	1:C:57:ARG:HD3	2.20	0.41
2:D:65:ALA:O	2:D:69:GLY:N	2.53	0.41
1:E:112:GLU:HB2	1:E:222:PRO:HA	2.03	0.41
2:H:27:ALA:HB1	2:H:29:TRP:CZ3	2.55	0.41
1:E:109:MET:CG	3:E:300:FAD:N7A	2.84	0.41
1:A:16:LEU:HD11	1:A:37:LEU:HD13	2.03	0.40
1:A:261:TYR:CD1	1:A:261:TYR:N	2.89	0.40
1:G:279:GLU:O	1:G:283:THR:HG23	2.21	0.40
3:G:301:FAD:H9	3:G:301:FAD:H1'1	1.92	0.40
1:C:122:LYS:HA	1:C:128:VAL:CG1	2.51	0.40
1:C:54:TYR:CD1	1:C:54:TYR:C	2.95	0.40
1:A:122:LYS:CD	1:A:130:TYR:HE2	2.35	0.40
2:B:78:ILE:O	2:B:84:PRO:HD2	2.22	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	275/288 (96%)	263 (96%)	11 (4%)	1 (0%)	34	64
1	C	274/288 (95%)	264 (96%)	9 (3%)	1 (0%)	34	64
1	E	275/288 (96%)	263 (96%)	10 (4%)	2 (1%)	22	52
1	G	276/288 (96%)	269 (98%)	6 (2%)	1 (0%)	34	64
2	B	87/108 (81%)	84 (97%)	2 (2%)	1 (1%)	14	40
2	D	89/108 (82%)	85 (96%)	4 (4%)	0	100	100
2	F	84/108 (78%)	80 (95%)	4 (5%)	0	100	100
2	H	74/108 (68%)	71 (96%)	3 (4%)	0	100	100
All	All	1434/1584 (90%)	1379 (96%)	49 (3%)	6 (0%)	34	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	259	LYS
1	E	259	LYS
1	G	259	LYS
1	E	116	PRO
2	B	74	PRO
1	A	259	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/237 (81%)	192 (100%)	0	100	100
1	C	202/237 (85%)	202 (100%)	0	100	100
1	E	166/237 (70%)	166 (100%)	0	100	100
1	G	162/237 (68%)	162 (100%)	0	100	100
2	B	54/94 (57%)	54 (100%)	0	100	100
2	D	53/94 (56%)	53 (100%)	0	100	100
2	F	42/94 (45%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	43/94 (46%)	43 (100%)	0	100	100
All	All	914/1324 (69%)	914 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
4	EDO	C	302	-	3,3,3	0.48	0	2,2,2	0.28	0
3	FAD	G	301	1	53,58,58	3.82	15 (28%)	68,89,89	2.00	17 (25%)
3	FAD	E	300	1	53,58,58	3.85	19 (35%)	68,89,89	1.95	16 (23%)
3	FAD	A	300	-	53,58,58	2.05	20 (37%)	68,89,89	2.11	25 (36%)
4	EDO	G	302	-	3,3,3	0.47	0	2,2,2	0.32	0
3	FAD	C	301	-	53,58,58	1.24	6 (11%)	68,89,89	1.42	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	302	-	-	0/1/1/1	-
3	FAD	G	301	1	-	3/30/50/50	0/6/6/6
3	FAD	E	300	1	-	3/30/50/50	0/6/6/6
3	FAD	A	300	-	-	6/30/50/50	0/6/6/6
4	EDO	G	302	-	-	1/1/1/1	-
3	FAD	C	301	-	-	14/30/50/50	0/6/6/6

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	FAD	C2B-C1B	-17.58	1.27	1.53
3	E	300	FAD	C2B-C1B	-17.42	1.27	1.53
3	E	300	FAD	O4B-C1B	15.61	1.62	1.41
3	G	301	FAD	O4B-C1B	15.39	1.62	1.41
3	E	300	FAD	C4X-N5	7.17	1.44	1.30
3	G	301	FAD	C4X-N5	6.65	1.43	1.30
3	E	300	FAD	O4B-C4B	-5.16	1.33	1.45
3	G	301	FAD	O4B-C4B	-5.15	1.33	1.45
3	G	301	FAD	C10-N1	4.89	1.43	1.33
3	C	301	FAD	C9A-C5X	4.85	1.49	1.41
3	E	300	FAD	C10-N1	4.84	1.43	1.33
3	A	300	FAD	C4-N3	-4.40	1.30	1.38
3	A	300	FAD	C2B-C1B	-4.24	1.47	1.53
3	A	300	FAD	C4A-N3A	-4.21	1.29	1.35
3	A	300	FAD	C4'-C3'	-4.18	1.45	1.53
3	G	301	FAD	C2-N1	4.05	1.46	1.36
3	E	300	FAD	C2-N1	4.04	1.46	1.36
3	G	301	FAD	C10-N10	3.78	1.45	1.37
3	A	300	FAD	C2-N3	-3.74	1.30	1.39
3	E	300	FAD	C2-N3	3.70	1.47	1.39
3	G	301	FAD	C2-N3	3.62	1.47	1.39
3	E	300	FAD	C10-N10	3.42	1.44	1.37
3	E	300	FAD	C2A-N3A	3.40	1.37	1.32
3	G	301	FAD	C2A-N3A	3.35	1.37	1.32
3	G	301	FAD	C9A-N10	3.31	1.47	1.41
3	A	300	FAD	C5X-N5	-3.22	1.33	1.39
3	A	300	FAD	C5A-N7A	-3.21	1.28	1.39
3	C	301	FAD	C8-C7	3.01	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	300	FAD	C9A-N10	2.89	1.46	1.41
3	A	300	FAD	C9A-C5X	2.86	1.46	1.41
3	E	300	FAD	C5X-N5	2.76	1.44	1.39
3	A	300	FAD	O4'-C4'	-2.75	1.37	1.43
3	A	300	FAD	P-O2P	-2.63	1.43	1.55
3	C	301	FAD	C4-N3	-2.61	1.34	1.38
3	A	300	FAD	PA-O2A	-2.48	1.43	1.55
3	A	300	FAD	PA-O1A	-2.44	1.42	1.50
3	A	300	FAD	C2'-C3'	-2.39	1.49	1.53
3	G	301	FAD	C2A-N1A	2.39	1.38	1.33
3	E	300	FAD	C2A-N1A	2.37	1.38	1.33
3	A	300	FAD	O2'-C2'	-2.36	1.38	1.43
3	G	301	FAD	C5A-C4A	-2.33	1.34	1.40
3	A	300	FAD	C1'-C2'	-2.31	1.49	1.52
3	A	300	FAD	C2B-C3B	-2.30	1.47	1.53
3	A	300	FAD	O4B-C4B	-2.27	1.39	1.45
3	E	300	FAD	C5A-C4A	-2.26	1.34	1.40
3	A	300	FAD	C6-C7	-2.25	1.36	1.39
3	G	301	FAD	C5X-N5	2.24	1.43	1.39
3	A	300	FAD	P-O1P	-2.23	1.43	1.50
3	C	301	FAD	C4X-N5	2.20	1.35	1.30
3	A	300	FAD	C2A-N1A	-2.20	1.29	1.33
3	E	300	FAD	O3B-C3B	-2.18	1.37	1.43
3	G	301	FAD	O3B-C3B	-2.16	1.37	1.43
3	E	300	FAD	C4A-N3A	2.15	1.38	1.35
3	E	300	FAD	C4-N3	2.15	1.42	1.38
3	G	301	FAD	C4A-N3A	2.13	1.38	1.35
3	C	301	FAD	C5A-C4A	2.12	1.46	1.40
3	C	301	FAD	C5X-N5	-2.10	1.35	1.39
3	E	300	FAD	C6-C7	2.09	1.42	1.39
3	E	300	FAD	C7M-C7	2.07	1.55	1.51
3	E	300	FAD	C2B-C3B	2.07	1.59	1.53

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	FAD	C7M-C7-C6	-6.70	107.10	119.49
3	E	300	FAD	C7M-C7-C6	-6.65	107.20	119.49
3	G	301	FAD	C7M-C7-C8	6.25	133.54	120.74
3	E	300	FAD	C7M-C7-C8	6.18	133.40	120.74
3	G	301	FAD	C5A-C6A-N6A	5.53	128.75	120.35
3	G	301	FAD	N3A-C2A-N1A	-5.39	120.26	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	300	FAD	C5A-C6A-N6A	5.36	128.50	120.35
3	E	300	FAD	N3A-C2A-N1A	-5.27	120.43	128.68
3	A	300	FAD	C4X-C10-N1	-4.98	113.16	124.73
3	A	300	FAD	P-O3P-PA	-4.92	115.94	132.83
3	C	301	FAD	P-O3P-PA	-4.46	117.53	132.83
3	A	300	FAD	C10-N1-C2	4.18	125.27	116.90
3	A	300	FAD	N3A-C2A-N1A	-4.11	122.25	128.68
3	A	300	FAD	C4-N3-C2	-4.03	118.19	125.64
3	A	300	FAD	O4B-C1B-C2B	-3.87	101.27	106.93
3	C	301	FAD	N3A-C2A-N1A	-3.80	122.74	128.68
3	A	300	FAD	O3'-C3'-C4'	-3.67	99.94	108.81
3	G	301	FAD	N6A-C6A-N1A	-3.48	111.35	118.57
3	E	300	FAD	N6A-C6A-N1A	-3.43	111.45	118.57
3	G	301	FAD	C4-N3-C2	-3.37	119.42	125.64
3	E	300	FAD	C3B-C2B-C1B	3.30	105.94	100.98
3	A	300	FAD	C4X-C4-N3	3.24	121.41	113.19
3	E	300	FAD	C4-N3-C2	-3.22	119.68	125.64
3	A	300	FAD	O4-C4-C4X	-3.06	118.49	126.60
3	C	301	FAD	C4X-C10-N1	-3.03	117.70	124.73
3	A	300	FAD	O4'-C4'-C3'	-2.91	102.02	109.10
3	E	300	FAD	C4X-C10-N10	2.87	120.67	116.48
3	A	300	FAD	C4X-C10-N10	2.86	120.67	116.48
3	G	301	FAD	C3B-C2B-C1B	2.78	105.16	100.98
3	G	301	FAD	C4-C4X-C10	2.74	121.39	116.79
3	A	300	FAD	C5A-C6A-N6A	-2.73	116.21	120.35
3	A	300	FAD	N10-C10-N1	2.72	126.17	118.35
3	A	300	FAD	C9A-N10-C10	-2.72	116.53	120.77
3	G	301	FAD	C4'-C3'-C2'	-2.71	107.73	113.36
3	C	301	FAD	C4A-C5A-N7A	-2.69	106.59	109.40
3	G	301	FAD	C4X-C10-N10	2.68	120.39	116.48
3	A	300	FAD	C8M-C8-C9	2.58	124.26	119.49
3	E	300	FAD	C4X-C4-N3	2.58	119.74	113.19
3	A	300	FAD	O3B-C3B-C4B	-2.57	103.62	111.05
3	A	300	FAD	N6A-C6A-N1A	2.55	123.87	118.57
3	G	301	FAD	C4X-C10-N1	-2.50	118.92	124.73
3	C	301	FAD	C10-N1-C2	2.50	121.90	116.90
3	E	300	FAD	C10-C4X-N5	-2.46	119.64	124.86
3	A	300	FAD	C8M-C8-C7	-2.45	115.71	120.74
3	G	301	FAD	C5X-C9A-N10	2.45	120.48	117.95
3	G	301	FAD	C8M-C8-C7	-2.44	115.74	120.74
3	G	301	FAD	C4X-C4-N3	2.42	119.33	113.19
3	C	301	FAD	O4-C4-C4X	-2.40	120.23	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	300	FAD	O4-C4-C4X	-2.40	120.23	126.60
3	A	300	FAD	C5X-C9A-N10	2.40	120.43	117.95
3	G	301	FAD	P-O3P-PA	-2.38	124.65	132.83
3	C	301	FAD	C4-C4X-N5	2.36	121.59	118.23
3	A	300	FAD	O2P-P-O1P	2.35	123.87	112.24
3	E	300	FAD	P-O3P-PA	-2.32	124.87	132.83
3	C	301	FAD	C4X-C4-N3	2.29	119.02	113.19
3	G	301	FAD	O4-C4-C4X	-2.27	120.57	126.60
3	C	301	FAD	C4-N3-C2	-2.26	121.47	125.64
3	A	300	FAD	C7M-C7-C6	2.23	123.62	119.49
3	G	301	FAD	C8M-C8-C9	2.22	123.59	119.49
3	A	300	FAD	O2'-C2'-C3'	-2.22	103.71	109.10
3	A	300	FAD	N3-C2-N1	2.19	123.68	119.38
3	E	300	FAD	C8M-C8-C7	-2.15	116.34	120.74
3	A	300	FAD	C1B-N9A-C4A	2.15	130.41	126.64
3	E	300	FAD	C10-N1-C2	2.14	121.18	116.90
3	C	301	FAD	C3B-C2B-C1B	2.14	104.20	100.98
3	C	301	FAD	C4X-C10-N10	2.13	119.60	116.48
3	E	300	FAD	C4X-C10-N1	-2.12	119.82	124.73
3	E	300	FAD	C8M-C8-C9	2.10	123.36	119.49
3	A	300	FAD	C9-C9A-C5X	-2.09	116.16	120.11
3	C	301	FAD	C2A-N1A-C6A	2.05	122.26	118.75

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	FAD	C5B-O5B-PA-O1A
3	A	300	FAD	C5B-O5B-PA-O2A
3	A	300	FAD	O4B-C4B-C5B-O5B
3	A	300	FAD	C3B-C4B-C5B-O5B
3	C	301	FAD	C5B-O5B-PA-O1A
3	C	301	FAD	C2'-C1'-N10-C10
3	C	301	FAD	C1'-C2'-C3'-O3'
3	C	301	FAD	C1'-C2'-C3'-C4'
3	C	301	FAD	O4'-C4'-C5'-O5'
3	C	301	FAD	C5'-O5'-P-O2P
3	E	300	FAD	C5B-O5B-PA-O1A
3	G	301	FAD	C5B-O5B-PA-O1A
3	C	301	FAD	O2'-C2'-C3'-O3'
3	C	301	FAD	O2'-C2'-C3'-C4'
3	C	301	FAD	C3'-C4'-C5'-O5'

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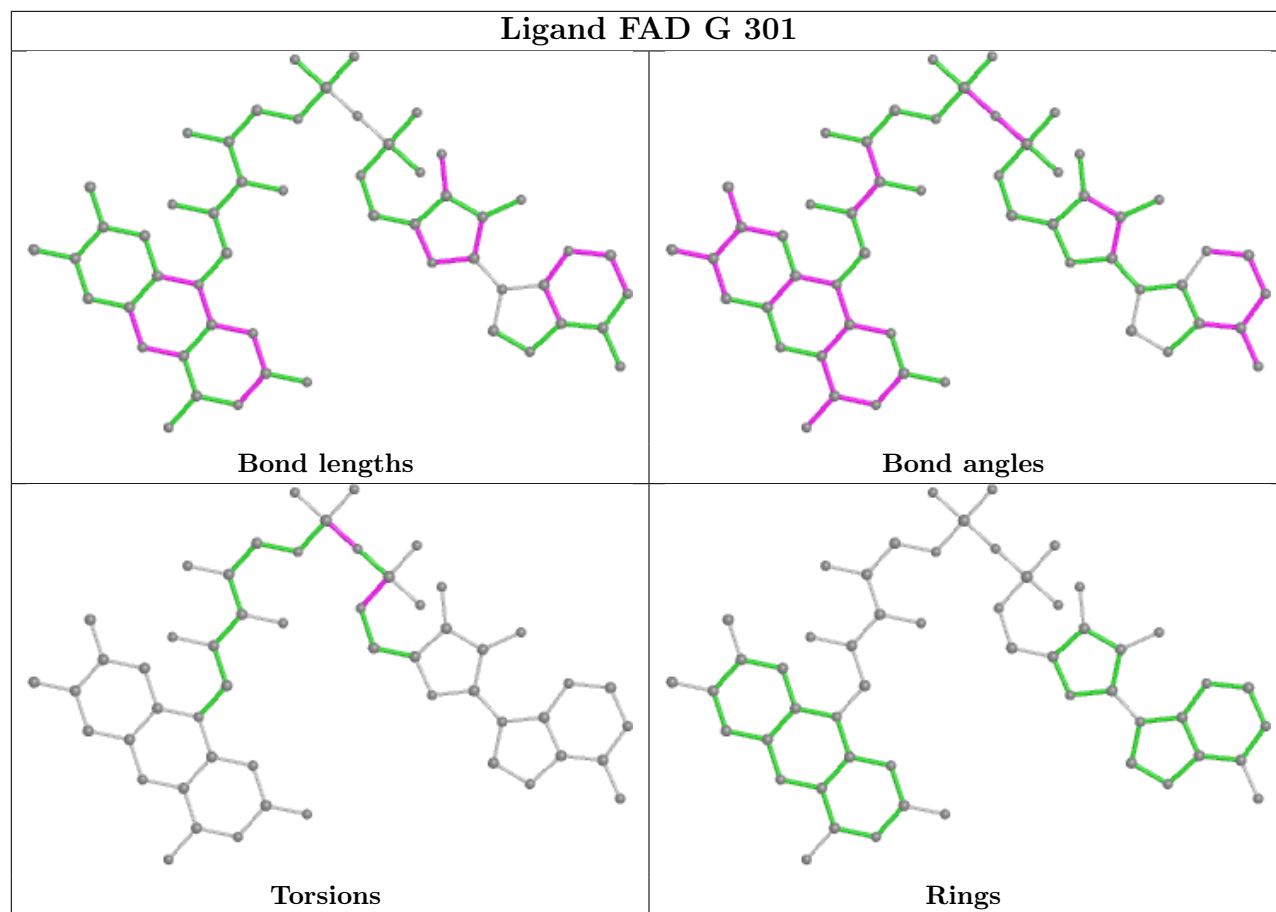
Mol	Chain	Res	Type	Atoms
3	C	301	FAD	PA-O3P-P-O5'
3	E	300	FAD	PA-O3P-P-O5'
3	G	301	FAD	PA-O3P-P-O5'
3	C	301	FAD	C5B-O5B-PA-O3P
3	C	301	FAD	C5'-O5'-P-O3P
3	C	301	FAD	P-O3P-PA-O1A
3	C	301	FAD	C5'-O5'-P-O1P
3	A	300	FAD	C2'-C1'-N10-C10
3	A	300	FAD	C5B-O5B-PA-O3P
3	E	300	FAD	C5B-O5B-PA-O3P
3	G	301	FAD	C5B-O5B-PA-O3P
4	G	302	EDO	O1-C1-C2-O2

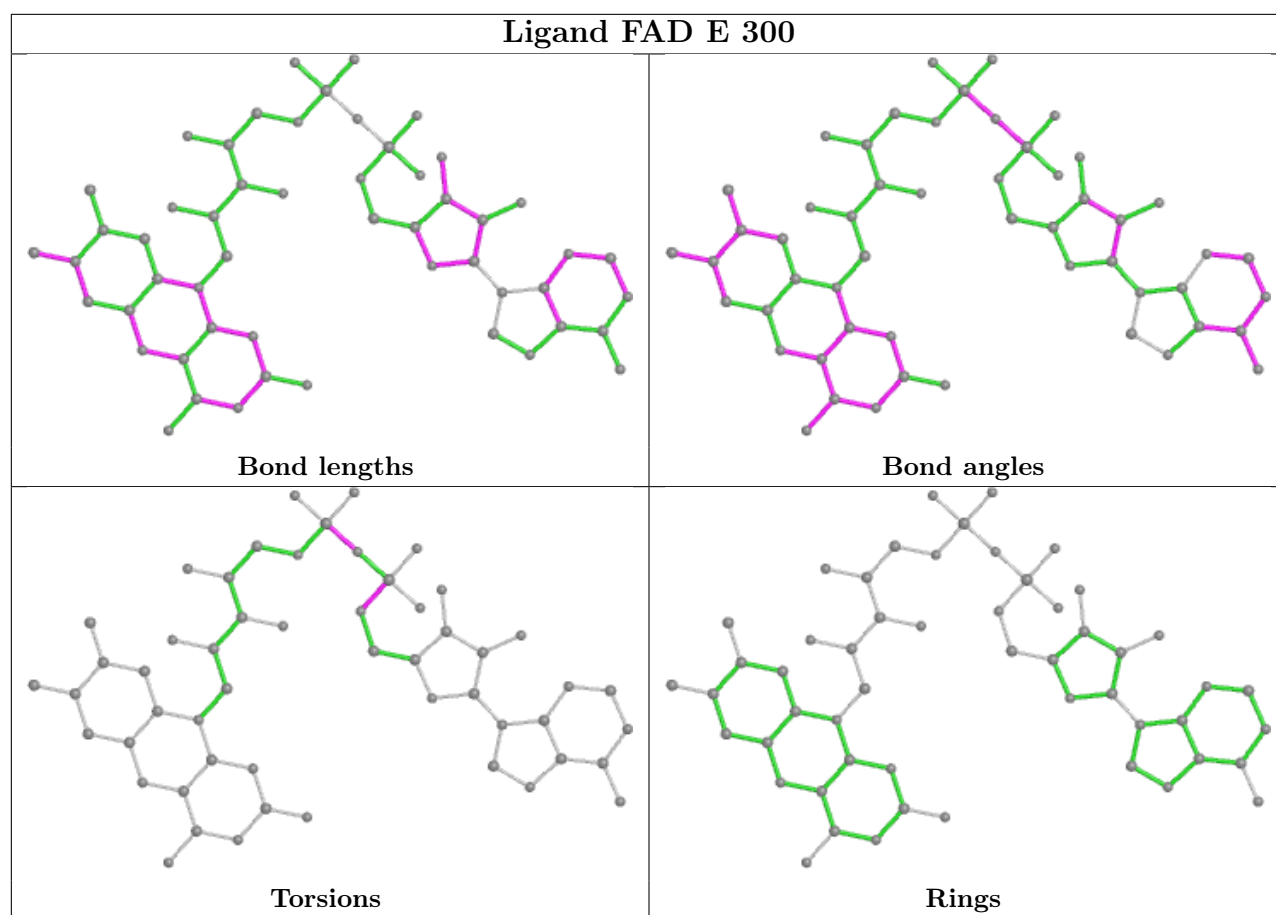
There are no ring outliers.

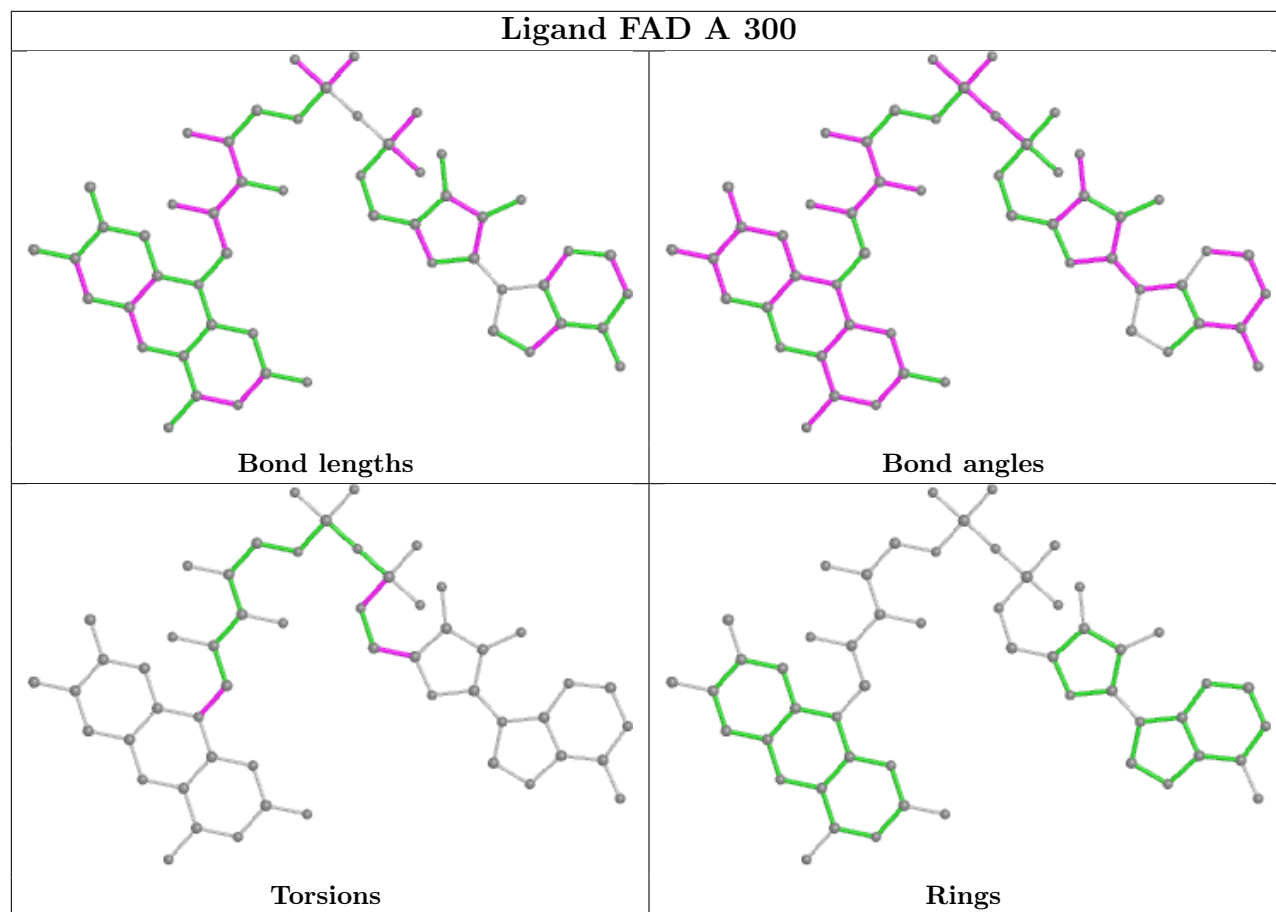
4 monomers are involved in 30 short contacts:

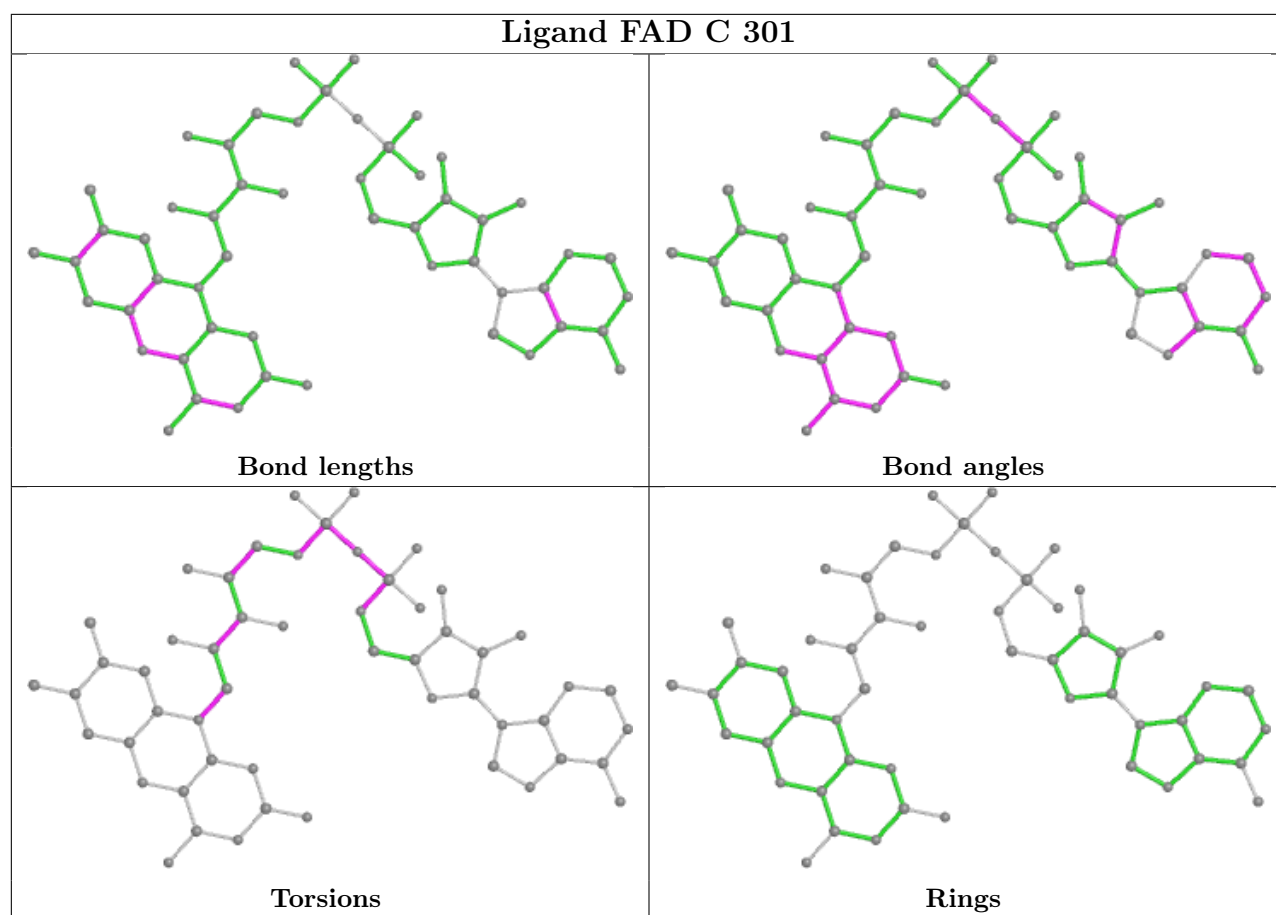
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	FAD	4	0
3	E	300	FAD	10	0
3	A	300	FAD	4	0
3	C	301	FAD	12	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/288 (96%)	0.32	9 (3%) 47 43	37, 68, 108, 137	0
1	C	278/288 (96%)	0.27	5 (1%) 68 67	42, 69, 106, 132	0
1	E	278/288 (96%)	0.27	14 (5%) 28 25	30, 82, 124, 143	0
1	G	280/288 (97%)	0.24	13 (4%) 32 28	35, 83, 130, 169	0
2	B	93/108 (86%)	0.12	4 (4%) 35 31	56, 108, 154, 186	0
2	D	95/108 (87%)	0.25	6 (6%) 20 16	58, 113, 175, 203	0
2	F	90/108 (83%)	-0.01	4 (4%) 34 30	71, 117, 159, 196	0
2	H	82/108 (75%)	0.14	5 (6%) 21 17	71, 121, 147, 175	0
All	All	1475/1584 (93%)	0.24	60 (4%) 37 32	30, 83, 138, 203	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	36	LEU	6.1
2	D	73	ILE	4.9
2	F	27	ALA	4.7
2	B	36	LEU	4.6
1	E	161	ALA	4.6
1	E	202	LEU	3.6
2	F	71	ALA	3.4
1	G	193	ILE	3.3
2	D	39	ILE	3.3
2	H	58	VAL	3.3
1	G	214	VAL	3.2
2	D	56	VAL	3.2
1	A	136	ALA	3.1
1	G	212	ASP	3.1
1	G	213	GLY	3.1
1	E	275	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	40	ILE	3.0
2	F	70	ILE	2.9
1	E	32	PHE	2.9
1	G	136	ALA	2.9
2	B	40	ILE	2.9
1	G	76	ILE	2.8
1	E	193	ILE	2.8
1	E	214	VAL	2.8
1	G	53	PHE	2.7
1	G	37	LEU	2.7
1	A	212	ASP	2.7
1	E	69	ILE	2.6
1	A	37	LEU	2.5
1	C	102	ALA	2.5
1	C	212	ASP	2.5
2	B	77	MET	2.4
1	E	194	VAL	2.4
1	G	69	ILE	2.4
1	C	84	ILE	2.4
1	A	6	ILE	2.4
1	G	32	PHE	2.4
1	A	74	ILE	2.4
1	E	76	ILE	2.3
1	C	1	MET	2.3
1	E	209	LEU	2.3
2	D	43	LEU	2.3
2	H	25	PHE	2.3
1	G	215	PHE	2.2
1	E	160	LEU	2.2
1	C	53	PHE	2.2
2	B	25	PHE	2.1
2	H	59	ASP	2.1
1	A	51	LEU	2.1
1	E	253	ALA	2.1
1	G	144	VAL	2.1
1	E	159	TYR	2.1
1	G	143	ILE	2.1
2	F	26	TRP	2.1
1	A	161	ALA	2.1
1	E	157	ALA	2.1
1	A	129	GLY	2.0
1	A	139	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	26	TRP	2.0
2	H	53	PHE	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](#)

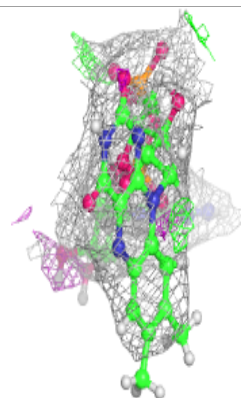
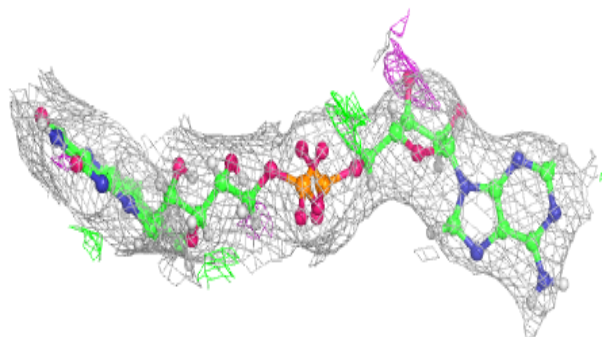
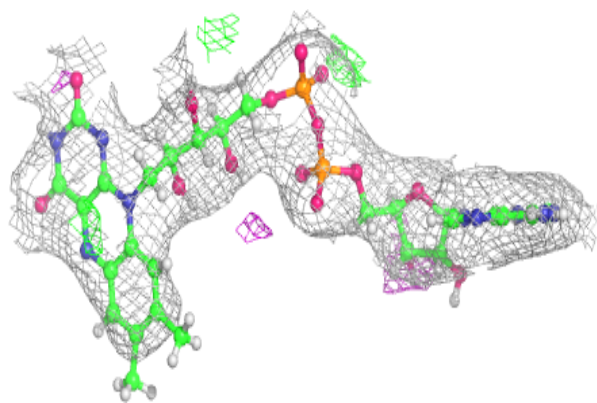
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	C	302	4/4	0.86	0.16	67,82,85,85	0
4	EDO	G	302	4/4	0.91	0.17	72,88,89,90	0
3	FAD	E	300	53/53	0.93	0.19	49,68,89,96	0
3	FAD	C	301	53/53	0.94	0.18	48,59,76,83	0
3	FAD	A	300	53/53	0.94	0.15	48,60,77,83	0
3	FAD	G	301	53/53	0.95	0.19	46,59,74,74	0

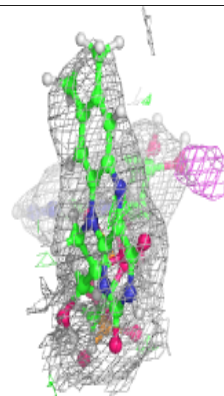
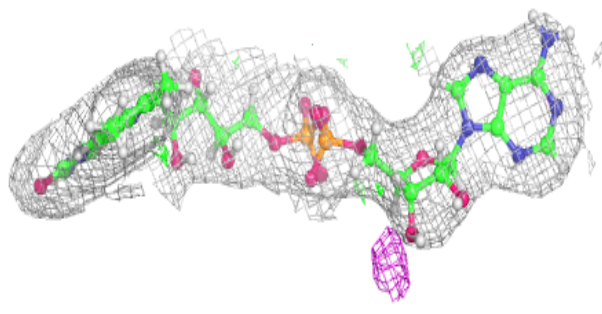
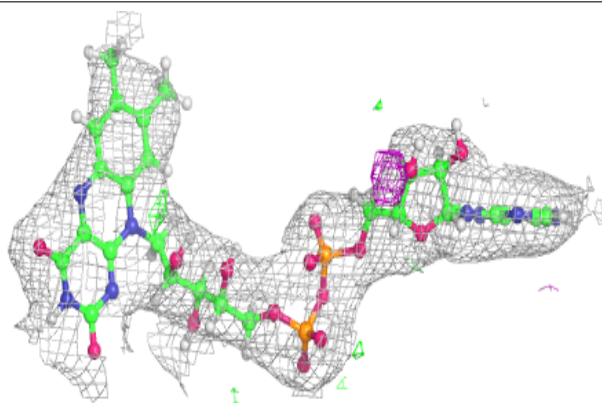
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD E 300:

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

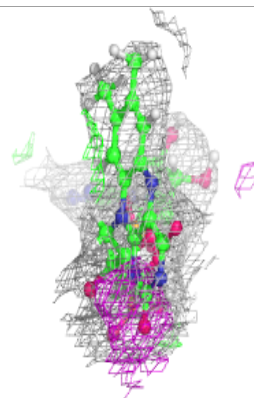
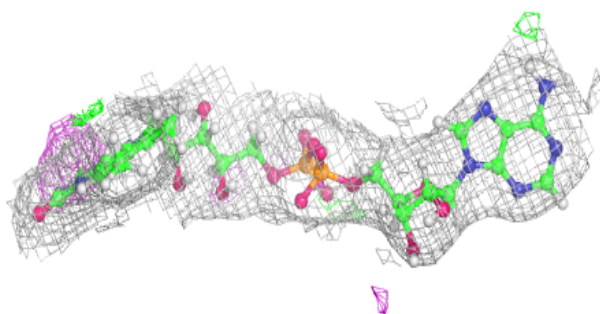
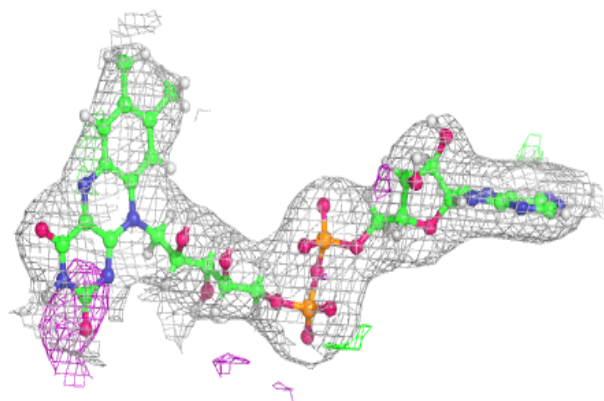
**Electron density around FAD C 301:**

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

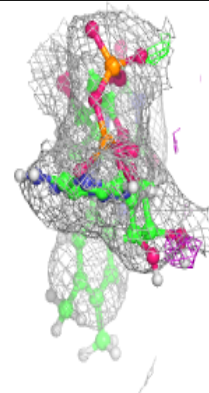
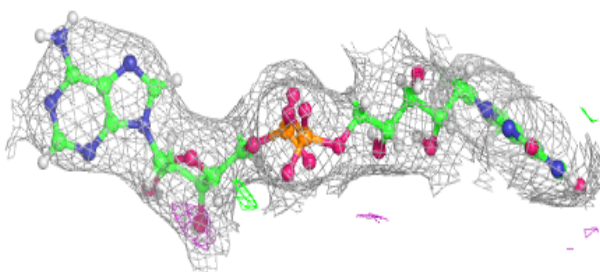
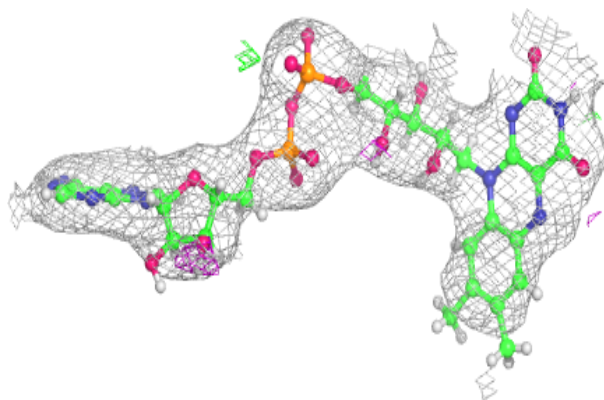


Electron density around FAD A 300:

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

**Electron density around FAD G 301:**

$2mF_o-DF_c$ (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.