



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:40 PM UTC

PDB ID : 3BG7 / pdb_00003bg7
Title : Pyranose 2-oxidase from Trametes multicolor, L537G mutant
Authors : Norberg, P.; Tan, T.C.; Divne, C.
Deposited on : 2007-11-26
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

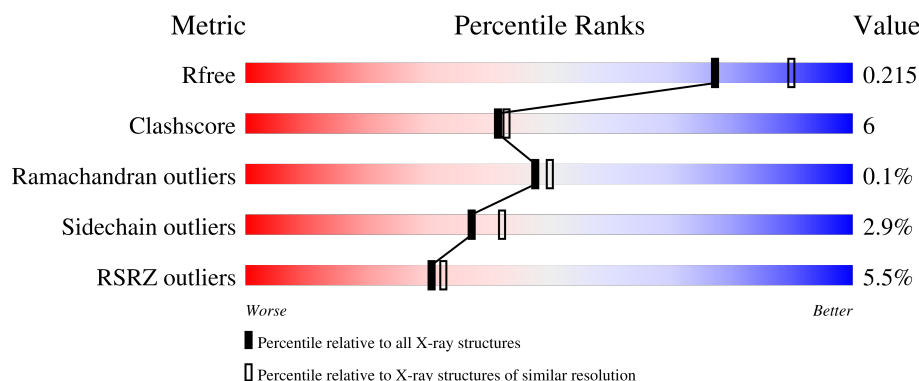
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	6% 81% 10% 7%
1	B	623	4% 81% 11% 7%
1	C	623	5% 80% 12% 7%
1	D	623	5% 82% 9% 7%
1	E	623	6% 82% 10% 7%

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Mol	Chain	Length	Quality of chain
1	F	623	5% 82% 9% 7%
1	G	623	4% 83% 8% 7%
1	H	623	5% 80% 12% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38641 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

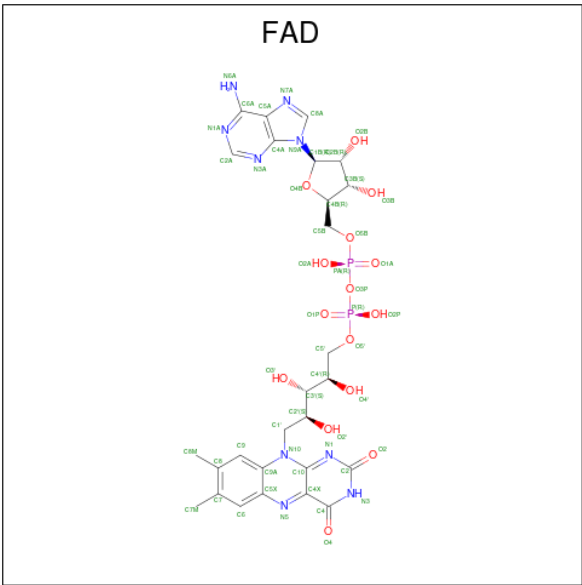
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	B	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	C	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	D	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	E	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	F	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	G	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	H	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	GLY	LEU	engineered mutation	UNP Q7ZA32
B	537	GLY	LEU	engineered mutation	UNP Q7ZA32
C	537	GLY	LEU	engineered mutation	UNP Q7ZA32
D	537	GLY	LEU	engineered mutation	UNP Q7ZA32
E	537	GLY	LEU	engineered mutation	UNP Q7ZA32
F	537	GLY	LEU	engineered mutation	UNP Q7ZA32
G	537	GLY	LEU	engineered mutation	UNP Q7ZA32
H	537	GLY	LEU	engineered mutation	UNP Q7ZA32

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	257	Total	O	0	0
			257	257		
3	B	279	Total	O	0	0
			279	279		
3	C	209	Total	O	0	0
			209	209		
3	D	231	Total	O	0	0
			231	231		

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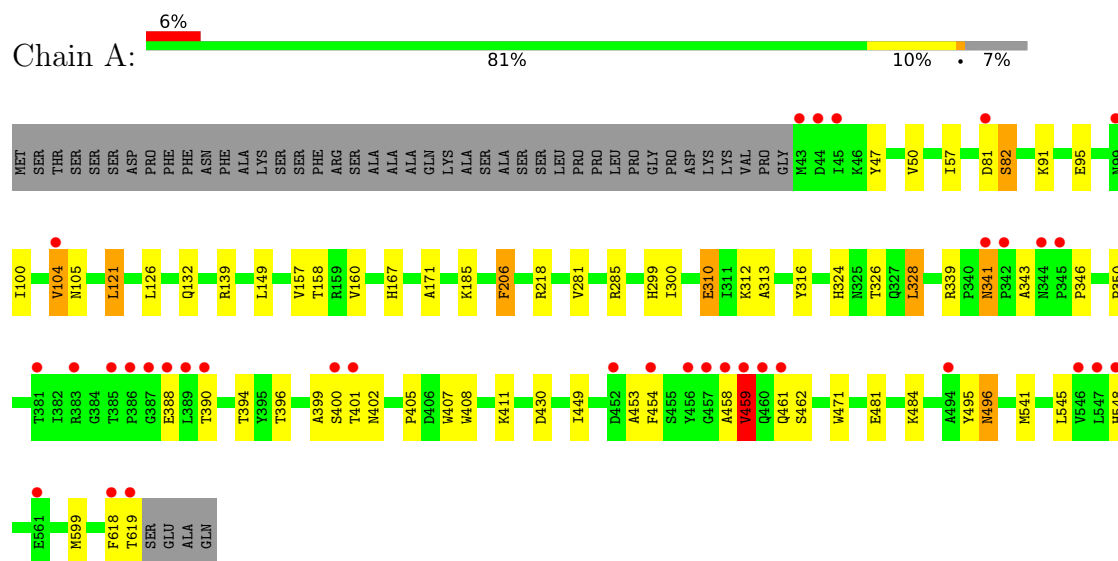
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	197	Total 197	O 197	0	0
3	F	197	Total 197	O 197	0	0
3	G	231	Total 231	O 231	0	0
3	H	256	Total 256	O 256	0	0

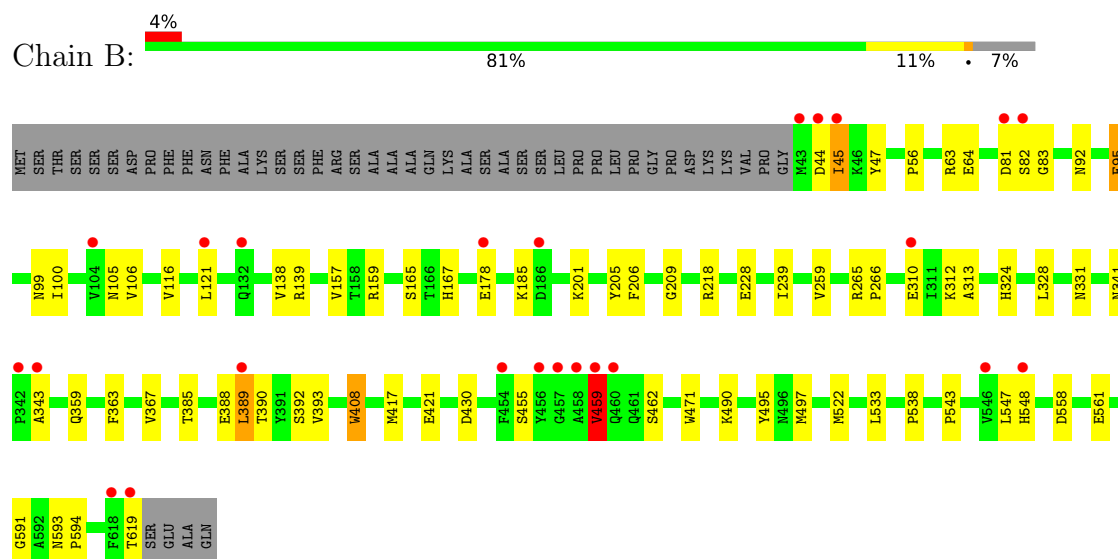
3 Residue-property plots [i](#)

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: Pyranose oxidase

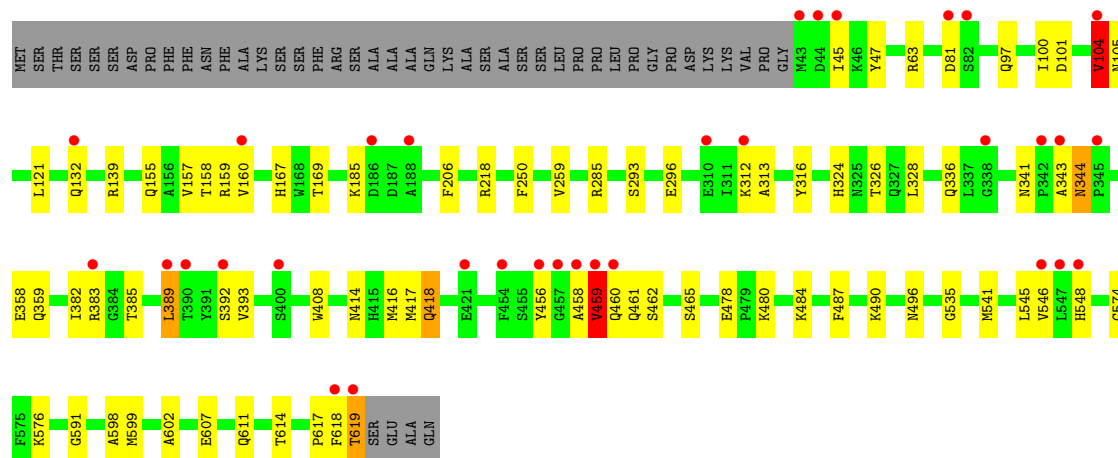


• Molecule 1: Pyranose oxidase



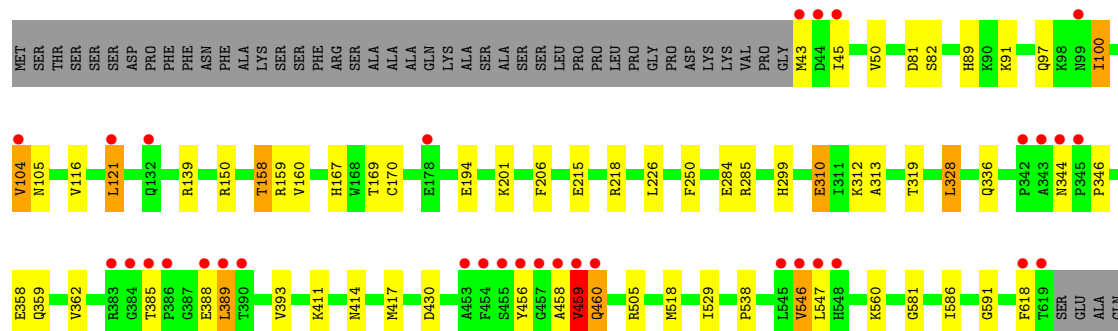
• Molecule 1: Pyranose oxidase

Chain C: 



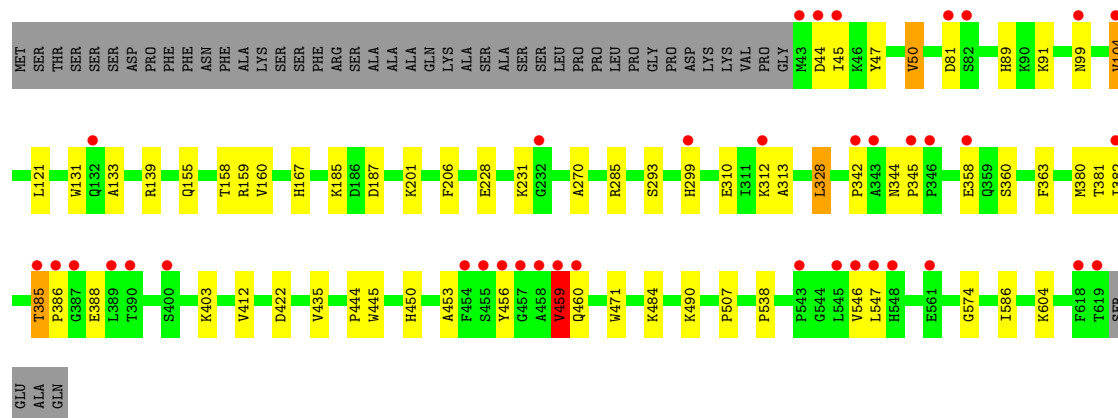
• Molecule 1: Pyranose oxidase

Chain D: 

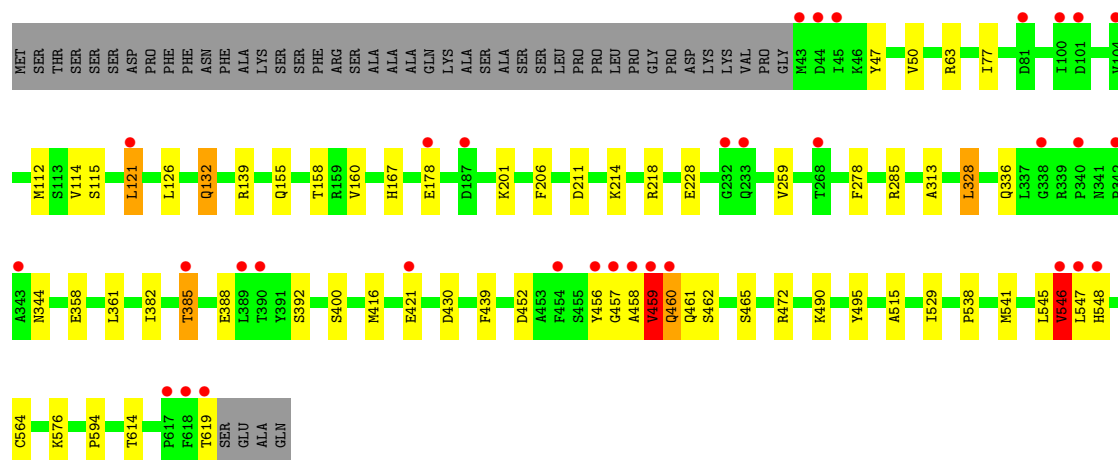
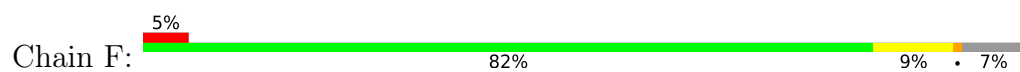


• Molecule 1: Pyranose oxidase

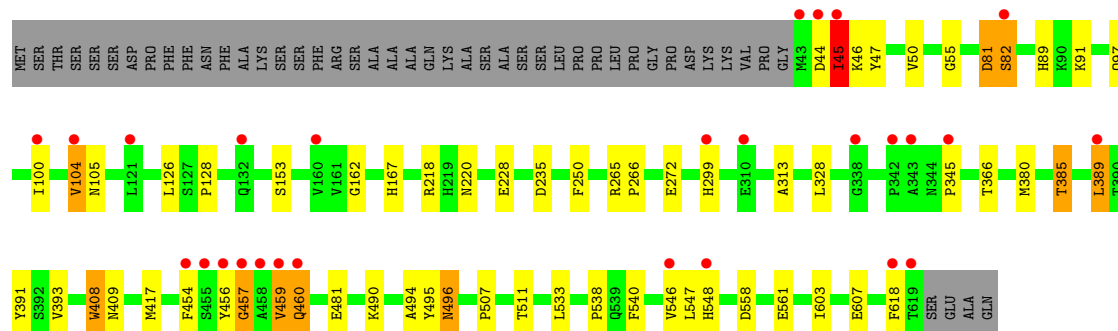
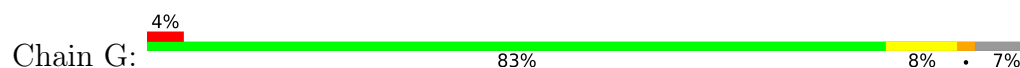
Chain E: 



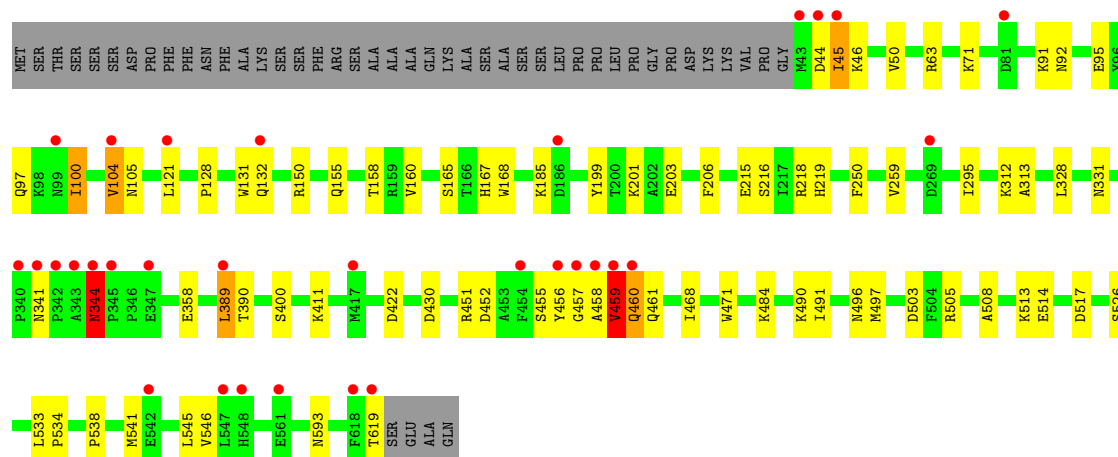
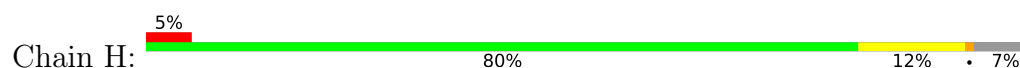
• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.54Å 103.18Å 169.34Å 90.00° 106.45° 90.00°	Depositor
Resolution (Å)	29.72 – 2.10 29.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.72-2.10) 99.0 (29.72-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.156 , 0.204 0.168 , 0.215	Depositor DCC
R_{free} test set	3262 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38641	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.34	10/4661 (0.2%)	1.11	9/6337 (0.1%)
1	B	1.32	6/4661 (0.1%)	1.11	7/6337 (0.1%)
1	C	1.18	6/4661 (0.1%)	1.07	6/6337 (0.1%)
1	D	1.22	11/4661 (0.2%)	1.08	8/6337 (0.1%)
1	E	1.17	7/4661 (0.2%)	1.06	8/6337 (0.1%)
1	F	1.14	5/4661 (0.1%)	1.05	9/6337 (0.1%)
1	G	1.26	9/4661 (0.2%)	1.10	7/6337 (0.1%)
1	H	1.23	7/4661 (0.2%)	1.11	8/6337 (0.1%)
All	All	1.23	61/37288 (0.2%)	1.09	62/50696 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	F	0	1
1	G	0	1
All	All	0	6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	450	HIS	C-O	-8.45	1.18	1.24
1	G	82	SER	N-CA	7.77	1.53	1.46
1	D	460	GLN	CA-C	7.03	1.62	1.52
1	D	81	ASP	CA-C	6.82	1.61	1.52
1	A	139	ARG	CD-NE	-6.62	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	114	VAL	C-O	-6.60	1.16	1.24
1	H	508	ALA	CA-CB	6.59	1.63	1.53
1	A	149	LEU	C-O	-6.59	1.14	1.23
1	H	459	VAL	CA-CB	6.55	1.62	1.54
1	G	45	ILE	CA-CB	6.54	1.63	1.54
1	F	546	VAL	CA-CB	6.53	1.61	1.54
1	B	228	GLU	CG-CD	6.50	1.68	1.52
1	G	460	GLN	CA-C	6.41	1.61	1.52
1	B	459	VAL	CA-CB	6.29	1.63	1.54
1	D	158	THR	CA-CB	6.27	1.62	1.53
1	C	104	VAL	C-O	-6.18	1.16	1.24
1	A	104	VAL	C-O	-6.14	1.16	1.24
1	D	310	GLU	CG-CD	5.97	1.67	1.52
1	G	345	PRO	CA-C	5.79	1.55	1.51
1	D	121	LEU	C-O	-5.71	1.17	1.23
1	H	128	PRO	C-O	-5.68	1.16	1.24
1	B	138	VAL	N-CA	-5.60	1.40	1.46
1	G	460	GLN	CB-CG	5.58	1.69	1.52
1	D	546	VAL	CA-CB	5.54	1.61	1.54
1	C	535	GLY	C-O	-5.53	1.15	1.24
1	D	310	GLU	CB-CG	5.51	1.69	1.52
1	A	326	THR	C-O	-5.48	1.17	1.24
1	B	239	ILE	CA-C	5.47	1.59	1.52
1	G	540	PHE	C-O	-5.47	1.17	1.23
1	E	104	VAL	C-O	-5.46	1.17	1.24
1	H	514	GLU	C-O	-5.46	1.17	1.24
1	F	115	SER	N-CA	5.45	1.53	1.46
1	E	604	LYS	C-O	-5.43	1.17	1.24
1	C	598	ALA	CA-CB	5.43	1.61	1.53
1	B	209	GLY	N-CA	5.43	1.50	1.45
1	C	602	ALA	N-CA	5.42	1.53	1.46
1	F	132	GLN	CD-OE1	5.42	1.33	1.23
1	A	316	TYR	C-O	-5.42	1.17	1.24
1	A	459	VAL	CA-CB	5.38	1.61	1.54
1	A	81	ASP	CA-C	5.33	1.59	1.52
1	D	529	ILE	CA-C	-5.29	1.47	1.52
1	H	295	ILE	CA-CB	5.28	1.60	1.54
1	E	435	VAL	C-O	5.25	1.30	1.24
1	D	459	VAL	CA-CB	5.24	1.61	1.54
1	H	92	ASN	C-O	-5.21	1.17	1.24
1	A	57	ILE	N-CA	5.18	1.52	1.46
1	E	459	VAL	CA-CB	5.16	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	50	VAL	CA-CB	5.15	1.60	1.54
1	D	139	ARG	CD-NE	-5.15	1.39	1.46
1	C	139	ARG	CD-NE	-5.14	1.39	1.46
1	G	494	ALA	CA-CB	5.14	1.62	1.53
1	C	81	ASP	CA-C	5.12	1.59	1.52
1	H	422	ASP	C-O	-5.12	1.17	1.24
1	G	366	THR	CA-CB	5.11	1.63	1.53
1	A	171	ALA	CA-CB	-5.10	1.46	1.53
1	F	139	ARG	CD-NE	-5.10	1.39	1.46
1	D	586	ILE	C-O	-5.09	1.18	1.24
1	G	235	ASP	C-O	5.08	1.29	1.23
1	A	310	GLU	CB-CG	5.06	1.67	1.52
1	B	459	VAL	CA-C	5.01	1.59	1.52
1	E	507	PRO	C-O	5.01	1.29	1.23

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	104	VAL	CB-CA-C	-10.93	97.38	112.14
1	D	104	VAL	CB-CA-C	-9.88	98.80	112.14
1	A	139	ARG	NE-CZ-NH2	-8.62	111.44	119.20
1	F	139	ARG	NE-CZ-NH2	-8.35	111.69	119.20
1	C	104	VAL	CB-CA-C	-7.53	102.18	112.04
1	E	422	ASP	CA-C-N	-7.49	112.13	120.45
1	E	422	ASP	C-N-CA	-7.49	112.13	120.45
1	E	270	ALA	CA-C-N	7.46	127.48	119.28
1	E	270	ALA	C-N-CA	7.46	127.48	119.28
1	A	339	ARG	CA-C-N	-7.39	112.71	120.03
1	A	339	ARG	C-N-CA	-7.39	112.71	120.03
1	G	82	SER	CA-CB-OG	7.25	125.60	111.10
1	B	594	PRO	N-CA-C	7.22	124.02	114.27
1	A	139	ARG	CG-CD-NE	-6.95	96.71	112.00
1	B	139	ARG	NE-CZ-NH2	-6.94	112.96	119.20
1	B	82	SER	CB-CA-C	-6.85	100.46	111.28
1	H	458	ALA	CA-C-N	6.84	129.23	120.88
1	H	458	ALA	C-N-CA	6.84	129.23	120.88
1	G	46	LYS	N-CA-C	6.81	119.99	108.90
1	H	104	VAL	N-CA-CB	6.38	119.22	110.54
1	A	82	SER	CB-CA-C	-6.28	101.38	111.18
1	E	139	ARG	NE-CZ-NH2	-6.12	113.70	119.20
1	C	546	VAL	N-CA-C	6.03	117.50	110.62
1	C	139	ARG	NE-CZ-NH2	-6.03	113.77	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	278	PHE	CA-C-N	5.99	125.96	120.21
1	F	278	PHE	C-N-CA	5.99	125.96	120.21
1	F	594	PRO	N-CA-C	5.99	122.35	114.27
1	A	139	ARG	CD-NE-CZ	5.93	132.70	124.40
1	D	116	VAL	CA-C-N	-5.81	114.63	120.21
1	D	116	VAL	C-N-CA	-5.81	114.63	120.21
1	G	55	GLY	CA-C-N	5.79	125.65	119.28
1	G	55	GLY	C-N-CA	5.79	125.65	119.28
1	D	414	ASN	N-CA-C	5.76	117.23	111.07
1	F	564	CYS	N-CA-C	5.65	117.20	109.18
1	B	106	VAL	N-CA-C	-5.63	105.03	110.72
1	H	484	LYS	N-CA-C	5.61	118.22	109.52
1	B	116	VAL	CA-C-N	-5.53	114.90	120.21
1	B	116	VAL	C-N-CA	-5.53	114.90	120.21
1	C	484	LYS	N-CA-C	5.52	118.23	109.50
1	G	220	ASN	N-CA-C	5.49	117.26	111.28
1	H	131	TRP	O-C-N	5.39	129.34	123.04
1	D	139	ARG	CG-CD-NE	-5.38	100.17	112.00
1	G	162	GLY	N-CA-C	-5.36	108.25	115.21
1	D	139	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	F	529	ILE	N-CA-C	-5.30	107.60	111.90
1	H	92	ASN	N-CA-C	-5.24	106.73	113.02
1	F	614	THR	CA-C-N	-5.22	114.41	119.78
1	F	614	THR	C-N-CA	-5.22	114.41	119.78
1	D	310	GLU	CB-CG-CD	5.19	121.43	112.60
1	E	586	ILE	CA-C-N	5.16	126.28	119.84
1	E	586	ILE	C-N-CA	5.16	126.28	119.84
1	C	614	THR	CA-C-N	-5.12	114.68	119.85
1	C	614	THR	C-N-CA	-5.12	114.68	119.85
1	A	396	THR	CA-C-N	-5.12	114.45	119.92
1	A	396	THR	C-N-CA	-5.12	114.45	119.92
1	F	139	ARG	CG-CD-NE	-5.09	100.81	112.00
1	B	92	ASN	N-CA-C	-5.08	107.59	112.97
1	A	484	LYS	N-CA-C	5.04	117.47	109.50
1	G	153	SER	N-CA-C	-5.04	105.88	112.23
1	H	344	ASN	N-CA-C	5.03	120.93	109.81
1	E	484	LYS	N-CA-C	5.02	117.43	109.50
1	D	226	LEU	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	390	THR	Peptide
1	A	459	VAL	Peptide
1	B	459	VAL	Peptide
1	C	459	VAL	Peptide
1	F	459	VAL	Peptide
1	G	81	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4545	0	4387	59	0
1	B	4545	0	4387	80	0
1	C	4545	0	4387	70	0
1	D	4545	0	4387	59	0
1	E	4545	0	4387	66	0
1	F	4545	0	4387	58	0
1	G	4545	0	4387	59	0
1	H	4545	0	4387	68	0
2	A	53	0	28	6	0
2	B	53	0	30	14	0
2	C	53	0	27	5	0
2	D	53	0	29	8	0
2	E	53	0	28	8	0
2	F	53	0	28	5	0
2	G	53	0	28	9	0
2	H	53	0	28	5	0
3	A	257	0	0	4	0
3	B	279	0	0	5	0
3	C	209	0	0	4	0
3	D	231	0	0	2	0
3	E	197	0	0	3	0
3	F	197	0	0	1	0
3	G	231	0	0	6	0
3	H	256	0	0	3	0
All	All	38641	0	35322	452	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 6.

All (452) 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:B:167:HIS:HE2	2:B:801:FAD:C8M	1.09	1.62
1:C:167:HIS:HE2	2:C:801:FAD:C8M	0.99	1.62
1:H:167:HIS:HE2	2:H:801:FAD:C8M	1.05	1.58
1:F:167:HIS:HE2	2:F:801:FAD:C8M	1.07	1.56
1:A:167:HIS:HE2	2:A:801:FAD:C8M	1.14	1.55
1:E:167:HIS:HE2	2:E:801:FAD:C8M	1.15	1.54
1:G:167:HIS:HE2	2:G:801:FAD:C8M	1.19	1.52
1:D:167:HIS:HE2	2:D:801:FAD:C8M	1.26	1.48
1:E:167:HIS:NE2	2:E:801:FAD:HM82	1.29	1.48
1:A:167:HIS:NE2	2:A:801:FAD:HM82	1.25	1.41
1:B:167:HIS:NE2	2:B:801:FAD:HM82	1.30	1.40
1:F:167:HIS:NE2	2:F:801:FAD:HM82	1.07	1.39
1:G:167:HIS:NE2	2:G:801:FAD:HM82	1.34	1.37
1:H:167:HIS:NE2	2:H:801:FAD:HM82	1.09	1.37
1:C:167:HIS:NE2	2:C:801:FAD:HM82	1.02	1.33
1:E:459:VAL:CG1	1:F:121:LEU:HD22	1.61	1.31
1:D:167:HIS:NE2	2:D:801:FAD:HM82	1.43	1.30
1:B:388:GLU:OE1	1:B:389:LEU:HD13	1.42	1.16
1:B:388:GLU:OE1	1:B:389:LEU:CD1	1.96	1.12
1:G:456:TYR:CD1	1:G:460:GLN:HB3	1.83	1.12
1:D:299:HIS:HB2	1:D:310:GLU:OE1	1.49	1.11
1:A:121:LEU:HD22	1:B:459:VAL:CG1	1.83	1.09
1:A:167:HIS:HE2	2:A:801:FAD:HM81	1.16	1.09
1:D:389:LEU:H	1:D:389:LEU:CD1	1.67	1.07
1:A:167:HIS:CD2	2:A:801:FAD:HM82	1.90	1.06
1:C:167:HIS:CD2	2:C:801:FAD:HM82	1.91	1.06
1:B:393:VAL:H	1:B:417:MET:HE1	1.21	1.02
1:D:389:LEU:H	1:D:389:LEU:HD12	0.86	1.01
1:D:389:LEU:HD12	1:D:389:LEU:N	1.71	1.00
1:E:459:VAL:HG11	1:F:121:LEU:HD22	1.00	0.98
1:C:167:HIS:HE2	2:C:801:FAD:HM81	1.29	0.98
1:F:167:HIS:CD2	2:F:801:FAD:HM82	1.99	0.97
1:D:167:HIS:HE2	2:D:801:FAD:HM81	1.30	0.96
1:A:459:VAL:HG13	1:B:121:LEU:HB3	1.47	0.96
1:A:121:LEU:HD22	1:B:459:VAL:HG11	1.43	0.96
1:A:121:LEU:HB3	1:B:459:VAL:CG1	1.96	0.95
1:D:167:HIS:HE2	2:D:801:FAD:HM82	0.82	0.95
1:E:459:VAL:HG11	1:F:121:LEU:CD2	1.96	0.95
1:C:121:LEU:HB3	1:D:459:VAL:CG1	1.96	0.95
1:C:121:LEU:HB3	1:D:459:VAL:HG13	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:393:VAL:H	1:G:417:MET:HE1	1.32	0.94
1:H:167:HIS:CD2	2:H:801:FAD:HM82	2.02	0.94
1:E:459:VAL:CG1	1:F:121:LEU:CD2	2.46	0.94
1:C:459:VAL:CG1	1:D:121:LEU:HB3	1.99	0.93
1:B:393:VAL:H	1:B:417:MET:CE	1.83	0.90
1:H:167:HIS:HE2	2:H:801:FAD:HM81	1.34	0.90
1:A:121:LEU:HB3	1:B:459:VAL:HG12	1.52	0.89
1:C:389:LEU:HD13	1:C:389:LEU:H	1.36	0.89
1:E:167:HIS:HE2	2:E:801:FAD:HM81	1.35	0.89
1:B:167:HIS:HE2	2:B:801:FAD:HM81	1.38	0.88
1:G:167:HIS:HE2	2:G:801:FAD:C8	1.87	0.87
1:A:121:LEU:HD22	1:B:459:VAL:HG13	1.57	0.87
1:H:341:ASN:HD22	1:H:344:ASN:CB	1.89	0.86
1:A:458:ALA:O	1:B:121:LEU:HD12	1.76	0.86
1:H:341:ASN:HD22	1:H:344:ASN:HB3	1.42	0.85
1:G:456:TYR:HD1	1:G:460:GLN:HB3	1.42	0.84
1:A:459:VAL:HG13	1:B:121:LEU:CB	2.07	0.84
1:B:167:HIS:HE2	2:B:801:FAD:HM82	0.68	0.84
1:E:121:LEU:CD2	1:H:121:LEU:CD2	2.57	0.83
1:B:167:HIS:HE2	2:B:801:FAD:C8	1.90	0.82
1:D:299:HIS:CB	1:D:310:GLU:OE1	2.26	0.82
1:F:167:HIS:HE2	2:F:801:FAD:HM81	1.43	0.82
1:A:341:ASN:HD22	1:A:343:ALA:H	1.28	0.81
1:A:459:VAL:CG1	1:B:121:LEU:HB3	2.11	0.81
1:G:167:HIS:HE2	2:G:801:FAD:HM82	0.63	0.80
1:F:285:ARG:HA	1:F:328:LEU:CD1	2.11	0.80
1:G:456:TYR:CD1	1:G:460:GLN:CB	2.65	0.80
1:C:459:VAL:HG13	1:D:121:LEU:HB3	1.64	0.80
1:E:167:HIS:HE2	2:E:801:FAD:HM82	0.64	0.80
1:E:167:HIS:CD2	2:E:801:FAD:HM82	2.16	0.80
1:E:459:VAL:HG13	1:F:121:LEU:HD22	1.64	0.79
1:C:121:LEU:CB	1:D:459:VAL:HG13	2.12	0.79
1:E:459:VAL:HG13	1:F:121:LEU:CG	2.13	0.79
1:D:167:HIS:CD2	2:D:801:FAD:HM82	2.17	0.79
1:B:388:GLU:OE1	1:B:389:LEU:HD11	1.81	0.78
1:F:541:MET:HE3	1:F:545:LEU:HD23	1.65	0.78
1:A:167:HIS:HE2	2:A:801:FAD:HM82	0.79	0.77
1:D:100:ILE:HD13	1:D:100:ILE:O	1.85	0.77
1:D:312:LYS:HE3	3:D:880:HOH:O	1.82	0.77
1:G:456:TYR:HD1	1:G:460:GLN:CB	1.97	0.77
1:C:478:GLU:OE2	1:C:480:LYS:HE2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ARG:HD2	1:F:259:VAL:O	1.85	0.76
1:D:393:VAL:H	1:D:417:MET:HE1	1.49	0.75
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.69	0.75
1:C:541:MET:HE2	1:C:545:LEU:HD23	1.68	0.74
1:B:389:LEU:HD13	1:B:389:LEU:H	1.53	0.74
1:H:541:MET:HE3	1:H:545:LEU:HD23	1.68	0.74
1:E:459:VAL:CG1	1:F:121:LEU:HB3	2.18	0.73
1:B:393:VAL:N	1:B:417:MET:HE1	2.00	0.73
1:E:121:LEU:HD22	1:H:121:LEU:CD2	2.18	0.73
1:A:285:ARG:HA	1:A:328:LEU:HD13	1.71	0.73
1:A:541:MET:HE3	1:A:545:LEU:HD23	1.69	0.73
1:D:285:ARG:HA	1:D:328:LEU:CD1	2.19	0.73
1:A:121:LEU:CD2	1:B:459:VAL:CG1	2.65	0.72
1:E:121:LEU:HB3	1:F:459:VAL:HG23	1.68	0.72
1:E:121:LEU:CD2	1:H:121:LEU:HD22	2.19	0.72
1:G:167:HIS:CE1	2:G:801:FAD:HM82	2.24	0.72
1:B:121:LEU:CD2	1:C:121:LEU:CD2	2.68	0.71
1:H:456:TYR:CD1	1:H:460:GLN:HB3	2.25	0.71
1:C:458:ALA:O	1:D:121:LEU:HD12	1.90	0.70
1:C:456:TYR:HB3	1:C:460:GLN:HB2	1.73	0.70
1:A:121:LEU:CB	1:B:459:VAL:CG1	2.70	0.69
1:H:460:GLN:HG2	1:H:533:LEU:HD21	1.73	0.69
1:C:459:VAL:O	1:C:462:SER:HB3	1.92	0.69
1:E:459:VAL:HG13	1:F:121:LEU:CD2	2.20	0.68
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.76	0.68
1:A:341:ASN:ND2	1:A:343:ALA:H	1.92	0.68
1:C:101:ASP:O	1:C:104:VAL:HG23	1.95	0.67
1:H:201:LYS:NZ	3:H:906:HOH:O	2.27	0.67
1:E:459:VAL:HG12	1:F:121:LEU:HB3	1.76	0.67
1:G:299:HIS:HB2	3:G:1133:HOH:O	1.94	0.67
1:D:285:ARG:HA	1:D:328:LEU:HD11	1.77	0.66
1:E:121:LEU:CB	1:F:459:VAL:HG23	2.26	0.66
1:E:299:HIS:HB2	1:E:310:GLU:OE1	1.96	0.66
1:C:359:GLN:NE2	1:C:591:GLY:O	2.29	0.66
1:A:121:LEU:CD2	1:B:459:VAL:HG13	2.24	0.66
1:C:617:PRO:O	1:C:619:THR:HG22	1.95	0.66
1:E:459:VAL:HG13	1:F:121:LEU:HD13	1.76	0.66
1:B:389:LEU:HD23	1:B:390:THR:HG23	1.77	0.66
1:H:619:THR:O	1:H:619:THR:HG23	1.95	0.66
1:B:121:LEU:HD21	1:C:121:LEU:CD2	2.26	0.66
1:B:121:LEU:CD2	1:C:121:LEU:HD21	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HD13	1:B:45:ILE:H	1.61	0.65
1:C:389:LEU:H	1:C:389:LEU:CD1	2.04	0.65
1:H:167:HIS:HE2	2:H:801:FAD:HM82	0.49	0.65
1:G:547:LEU:CD1	2:G:801:FAD:HM83	2.27	0.65
1:G:393:VAL:H	1:G:417:MET:CE	2.07	0.65
1:C:158:THR:HG22	1:C:160:VAL:HG22	1.78	0.65
1:D:359:GLN:NE2	1:D:591:GLY:O	2.30	0.65
1:B:167:HIS:NE2	2:B:801:FAD:C8	2.57	0.64
1:H:158:THR:HG22	1:H:160:VAL:HG22	1.80	0.64
1:E:121:LEU:HD22	1:H:121:LEU:HD21	1.80	0.64
1:C:459:VAL:HG13	1:D:121:LEU:CB	2.27	0.63
1:B:178:GLU:HG3	3:B:972:HOH:O	1.97	0.63
1:H:490:LYS:HD2	1:H:491:ILE:HD13	1.79	0.63
1:E:459:VAL:HG13	1:F:121:LEU:CD1	2.28	0.63
1:C:121:LEU:CB	1:D:459:VAL:CG1	2.73	0.63
1:B:45:ILE:H	1:B:45:ILE:CD1	2.12	0.63
1:E:91:LYS:NZ	3:E:822:HOH:O	2.30	0.63
1:E:121:LEU:HD21	1:H:121:LEU:HD22	1.81	0.62
1:E:121:LEU:HD12	1:F:458:ALA:O	1.99	0.62
1:C:344:ASN:HD22	1:C:344:ASN:N	1.98	0.62
1:B:389:LEU:CD2	1:B:390:THR:HG23	2.29	0.61
1:E:89:HIS:CE1	1:E:91:LYS:HG2	2.35	0.61
1:G:167:HIS:NE2	2:G:801:FAD:C8	2.54	0.61
1:H:389:LEU:HD23	1:H:390:THR:N	2.15	0.61
1:F:328:LEU:HD12	1:F:328:LEU:O	2.00	0.61
1:G:89:HIS:CE1	1:G:91:LYS:HB2	2.35	0.61
1:H:341:ASN:HD22	1:H:344:ASN:HB2	1.65	0.61
1:B:359:GLN:OE1	1:B:548:HIS:ND1	2.33	0.60
1:F:285:ARG:HA	1:F:328:LEU:HD11	1.82	0.60
1:C:459:VAL:CG1	1:D:121:LEU:CB	2.77	0.59
1:C:359:GLN:OE1	1:C:548:HIS:HB2	2.02	0.59
1:G:547:LEU:HD12	2:G:801:FAD:HM83	1.84	0.59
1:E:344:ASN:N	1:E:345:PRO:HD3	2.16	0.59
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.85	0.59
1:A:91:LYS:NZ	3:A:963:HOH:O	2.35	0.59
1:C:296:GLU:O	1:C:312:LYS:HD3	2.02	0.58
1:E:385:THR:HG22	1:E:386:PRO:HD2	1.85	0.58
1:C:343:ALA:C	1:C:344:ASN:HD22	2.11	0.58
1:C:389:LEU:HD13	1:C:389:LEU:N	2.15	0.58
1:H:91:LYS:NZ	3:H:980:HOH:O	2.35	0.58
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:HIS:CB	1:E:310:GLU:OE1	2.52	0.58
1:G:558:ASP:HB3	1:G:561:GLU:HB3	1.86	0.58
1:A:121:LEU:CG	1:B:459:VAL:HG13	2.34	0.58
1:F:459:VAL:O	1:F:462:SER:HB3	2.04	0.57
1:B:459:VAL:HA	1:B:462:SER:HB2	1.86	0.57
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.85	0.57
1:C:459:VAL:O	1:C:462:SER:CB	2.53	0.57
1:B:167:HIS:NE2	2:B:801:FAD:HM81	2.08	0.57
1:A:407:TRP:O	1:A:411:LYS:HG3	2.05	0.57
1:F:452:ASP:OD2	1:F:472:ARG:CZ	2.52	0.57
1:G:456:TYR:HD1	1:G:460:GLN:CG	2.17	0.57
1:G:82:SER:HB2	3:G:1013:HOH:O	2.05	0.57
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.05	0.56
1:G:460:GLN:HG3	1:G:533:LEU:HD21	1.86	0.56
1:B:547:LEU:HD12	2:B:801:FAD:HM83	1.87	0.56
1:D:201:LYS:NZ	3:D:881:HOH:O	2.28	0.56
1:E:104:VAL:CG2	1:E:453:ALA:HB1	2.35	0.56
1:F:47:TYR:O	1:F:313:ALA:HA	2.05	0.56
1:H:460:GLN:HG2	1:H:533:LEU:CD2	2.34	0.56
1:H:389:LEU:HD23	1:H:390:THR:HG23	1.87	0.56
1:E:104:VAL:HG23	1:E:453:ALA:HB1	1.87	0.55
1:A:121:LEU:CB	1:B:459:VAL:HG13	2.36	0.55
1:G:459:VAL:HG12	1:G:460:GLN:N	2.21	0.55
1:G:546:VAL:HG13	1:G:548:HIS:H	1.71	0.55
1:A:104:VAL:CG2	1:A:454:PHE:N	2.70	0.54
1:C:218:ARG:HD2	3:C:882:HOH:O	2.06	0.54
1:C:459:VAL:HG12	1:D:121:LEU:HB3	1.83	0.54
1:H:45:ILE:C	1:H:45:ILE:HD12	2.32	0.54
1:A:299:HIS:HD1	1:A:310:GLU:CD	2.14	0.54
1:B:201:LYS:NZ	3:B:952:HOH:O	2.40	0.54
1:C:158:THR:CG2	1:C:160:VAL:HG22	2.36	0.54
1:H:218:ARG:HG3	1:H:430:ASP:OD2	2.08	0.54
1:G:456:TYR:CG	1:G:460:GLN:HB3	2.41	0.54
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.90	0.54
1:G:481:GLU:HG2	3:G:1084:HOH:O	2.08	0.54
1:F:382:ILE:HD11	1:F:416:MET:HE1	1.89	0.54
1:B:167:HIS:CE1	2:B:801:FAD:HM82	2.28	0.53
1:C:293:SER:HA	1:C:574:GLY:O	2.08	0.53
1:C:121:LEU:HD12	1:D:458:ALA:O	2.08	0.53
1:D:456:TYR:HB3	1:D:460:GLN:HB2	1.91	0.53
1:B:81:ASP:OD1	1:B:81:ASP:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:HIS:ND1	1:G:91:LYS:HB2	2.23	0.53
1:G:44:ASP:OD1	1:G:45:ILE:N	2.42	0.53
1:A:104:VAL:HG21	1:A:454:PHE:CA	2.39	0.53
1:E:121:LEU:HB3	1:F:459:VAL:CG2	2.37	0.53
1:H:460:GLN:CG	1:H:533:LEU:HD21	2.38	0.53
1:E:459:VAL:CG1	1:F:121:LEU:CB	2.87	0.53
1:G:456:TYR:HD1	1:G:460:GLN:HG2	1.73	0.52
1:H:312:LYS:NZ	3:H:948:HOH:O	2.42	0.52
1:A:167:HIS:CD2	2:A:801:FAD:C8M	2.73	0.52
1:A:481:GLU:HG2	3:A:1028:HOH:O	2.08	0.52
1:C:47:TYR:O	1:C:313:ALA:HA	2.09	0.52
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.44	0.52
1:E:459:VAL:HG13	1:F:121:LEU:CB	2.39	0.52
1:F:361:LEU:HD23	1:F:541:MET:HG3	1.92	0.52
1:B:388:GLU:HB3	1:B:389:LEU:HD22	1.92	0.52
1:C:97:GLN:HG3	1:C:250:PHE:CD2	2.44	0.52
1:A:346:PRO:HG2	1:A:350:PRO:HA	1.92	0.52
1:E:285:ARG:HA	1:E:328:LEU:CD1	2.40	0.52
1:H:490:LYS:O	1:H:490:LYS:HD3	2.08	0.52
1:A:218:ARG:HG3	1:A:430:ASP:OD2	2.10	0.52
1:B:167:HIS:CD2	2:B:801:FAD:HM82	2.32	0.52
1:F:456:TYR:HB3	1:F:460:GLN:HB2	1.92	0.52
1:G:459:VAL:O	1:G:460:GLN:C	2.53	0.51
1:A:121:LEU:CD2	1:B:459:VAL:HG11	2.28	0.51
1:H:44:ASP:OD2	1:H:71:LYS:NZ	2.34	0.51
1:F:382:ILE:CD1	1:F:416:MET:HE1	2.41	0.51
1:H:619:THR:O	1:H:619:THR:CG2	2.59	0.51
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.92	0.51
1:F:459:VAL:O	1:F:462:SER:CB	2.59	0.51
1:D:89:HIS:ND1	1:D:91:LYS:HB3	2.26	0.51
1:G:457:GLY:C	1:G:459:VAL:H	2.19	0.50
1:E:459:VAL:CG1	1:F:121:LEU:CG	2.82	0.50
1:F:211:ASP:HB2	1:F:214:LYS:HD3	1.93	0.50
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.92	0.50
1:G:393:VAL:N	1:G:417:MET:HE1	2.14	0.50
1:B:167:HIS:CE1	2:B:801:FAD:C8M	2.88	0.50
1:B:331:ASN:ND2	1:B:497:MET:HE1	2.27	0.50
1:E:456:TYR:HD1	1:E:460:GLN:HB3	1.76	0.50
1:F:361:LEU:CD2	1:F:541:MET:HG3	2.42	0.50
1:H:471:TRP:CH2	1:H:526:SER:HA	2.47	0.50
1:G:104:VAL:HG21	1:G:454:PHE:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:HIS:C	1:G:167:HIS:CD2	2.89	0.50
1:A:104:VAL:HG22	1:A:453:ALA:C	2.37	0.49
1:C:169:THR:HG22	1:C:169:THR:O	2.12	0.49
1:H:451:ARG:HD3	1:H:468:ILE:O	2.12	0.49
1:C:132:GLN:NE2	3:C:930:HOH:O	2.44	0.49
1:B:167:HIS:CD2	1:B:167:HIS:C	2.90	0.49
1:D:336:GLN:HB2	1:D:346:PRO:HG3	1.95	0.49
1:E:342:PRO:C	1:E:344:ASN:H	2.20	0.49
1:G:495:TYR:OH	1:H:95:GLU:OE1	2.25	0.49
1:G:546:VAL:HG13	1:G:547:LEU:N	2.27	0.49
1:G:91:LYS:NZ	3:G:958:HOH:O	2.45	0.49
1:G:618:PHE:CD1	1:G:618:PHE:C	2.90	0.49
1:B:95:GLU:O	1:B:99:ASN:ND2	2.45	0.49
1:E:99:ASN:ND2	1:F:112:MET:SD	2.86	0.49
1:A:285:ARG:HA	1:A:328:LEU:CD1	2.41	0.49
1:A:341:ASN:HD22	1:A:341:ASN:C	2.21	0.49
1:H:344:ASN:CG	1:H:344:ASN:O	2.55	0.49
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.12	0.48
1:C:393:VAL:H	1:C:417:MET:HE1	1.76	0.48
1:C:408:TRP:CD1	1:C:408:TRP:C	2.90	0.48
1:C:617:PRO:O	1:C:619:THR:N	2.47	0.48
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.95	0.48
1:E:201:LYS:NZ	3:E:945:HOH:O	2.47	0.48
1:F:328:LEU:HD12	1:F:328:LEU:C	2.37	0.48
1:G:47:TYR:O	1:G:313:ALA:HA	2.14	0.48
1:B:341:ASN:OD1	1:B:343:ALA:HB3	2.14	0.48
1:C:285:ARG:HA	1:C:328:LEU:CD1	2.43	0.48
1:E:360:SER:HB2	3:E:998:HOH:O	2.14	0.48
1:F:201:LYS:NZ	3:F:964:HOH:O	2.46	0.48
1:F:619:THR:HG23	1:F:619:THR:O	2.13	0.48
1:H:63:ARG:HD2	1:H:259:VAL:O	2.14	0.48
1:H:100:ILE:C	1:H:100:ILE:HD13	2.39	0.48
1:A:95:GLU:OE1	1:B:495:TYR:OH	2.29	0.47
1:B:408:TRP:CD1	1:B:408:TRP:C	2.92	0.47
1:C:312:LYS:HD2	1:C:316:TYR:OH	2.13	0.47
1:C:343:ALA:C	1:C:344:ASN:ND2	2.73	0.47
1:D:150:ARG:NH1	1:D:505:ARG:HG3	2.29	0.47
1:B:558:ASP:HB3	1:B:561:GLU:HB2	1.96	0.47
1:D:393:VAL:H	1:D:417:MET:CE	2.22	0.47
1:E:344:ASN:N	1:E:345:PRO:CD	2.77	0.47
1:C:618:PHE:CD1	1:C:618:PHE:C	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:ASP:OD1	1:G:45:ILE:HG13	2.14	0.47
1:H:331:ASN:ND2	1:H:497:MET:HE1	2.30	0.47
1:G:507:PRO:HD2	1:G:511:THR:HG21	1.96	0.47
1:F:218:ARG:HG3	1:F:430:ASP:OD2	2.14	0.47
1:C:63:ARG:HD2	1:C:259:VAL:O	2.14	0.47
1:D:359:GLN:NE2	1:D:591:GLY:C	2.73	0.47
1:H:456:TYR:CD1	1:H:460:GLN:CB	2.95	0.47
1:H:341:ASN:ND2	1:H:344:ASN:CB	2.69	0.47
1:A:449:ILE:HG12	1:A:471:TRP:CE3	2.50	0.47
1:D:299:HIS:CA	1:D:310:GLU:OE1	2.62	0.47
1:E:546:VAL:HG13	1:E:547:LEU:N	2.30	0.47
1:A:47:TYR:O	1:A:313:ALA:HA	2.15	0.46
1:C:359:GLN:HE21	1:C:591:GLY:C	2.23	0.46
1:E:155:GLN:NE2	1:E:358:GLU:OE2	2.48	0.46
1:E:444:PRO:HD2	1:E:445:TRP:CZ3	2.50	0.46
1:B:121:LEU:HD22	1:C:121:LEU:HD21	1.96	0.46
1:C:100:ILE:CD1	3:C:989:HOH:O	2.63	0.46
1:D:336:GLN:NE2	1:D:344:ASN:O	2.47	0.46
1:G:546:VAL:CG1	1:G:547:LEU:N	2.78	0.46
1:A:405:PRO:O	1:A:408:TRP:HB3	2.15	0.46
1:C:618:PHE:C	1:C:618:PHE:HD1	2.24	0.46
1:E:293:SER:HA	1:E:574:GLY:O	2.15	0.46
1:G:408:TRP:CD1	1:G:408:TRP:C	2.93	0.46
1:F:126:LEU:HD13	1:F:132:GLN:CG	2.45	0.46
1:B:392:SER:HA	1:B:417:MET:HE1	1.98	0.46
1:B:459:VAL:O	1:B:462:SER:HB3	2.16	0.46
1:A:618:PHE:CD1	1:A:618:PHE:C	2.93	0.46
1:B:389:LEU:CD1	1:B:389:LEU:H	2.22	0.46
1:E:47:TYR:O	1:E:313:ALA:HA	2.15	0.46
1:H:100:ILE:HD13	1:H:100:ILE:O	2.15	0.46
1:H:456:TYR:HD1	1:H:460:GLN:CB	2.28	0.46
1:B:45:ILE:CD1	1:B:45:ILE:N	2.78	0.46
1:H:150:ARG:NH1	1:H:505:ARG:HG3	2.31	0.46
1:C:341:ASN:HD21	1:C:343:ALA:HB3	1.81	0.46
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.51	0.46
1:G:380:MET:HE1	1:G:409:ASN:HB3	1.98	0.46
1:A:206:PHE:CE2	1:A:599:MET:CE	2.99	0.46
1:C:206:PHE:CE2	1:C:599:MET:HE3	2.51	0.46
1:C:414:ASN:O	1:C:418:GLN:HG2	2.16	0.46
1:E:158:THR:HG22	1:E:160:VAL:HG22	1.99	0.46
1:H:155:GLN:NE2	1:H:358:GLU:OE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:PHE:CE2	1:C:599:MET:CE	2.99	0.45
1:D:89:HIS:CE1	1:D:91:LYS:HB3	2.51	0.45
1:H:45:ILE:C	1:H:45:ILE:CD1	2.89	0.45
1:A:399:ALA:O	1:A:402:ASN:HB2	2.16	0.45
1:D:169:THR:O	1:D:170:CYS:HB2	2.17	0.45
1:B:63:ARG:HD2	1:B:259:VAL:O	2.17	0.45
1:H:452:ASP:C	1:H:452:ASP:OD1	2.59	0.45
1:H:456:TYR:HD1	1:H:460:GLN:HB3	1.79	0.45
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.16	0.45
1:G:218:ARG:HD2	3:G:1014:HOH:O	2.15	0.45
1:B:159:ARG:HA	2:B:801:FAD:O2B	2.17	0.45
1:D:43:MET:HE3	1:D:45:ILE:HG22	1.99	0.45
1:E:131:TRP:CH2	1:E:133:ALA:HB2	2.52	0.44
1:E:328:LEU:C	1:E:328:LEU:HD12	2.42	0.44
1:A:126:LEU:CD1	1:A:132:GLN:CG	2.95	0.44
1:C:167:HIS:CD2	1:C:167:HIS:C	2.94	0.44
1:E:167:HIS:CD2	1:E:167:HIS:C	2.95	0.44
1:B:522:MET:HE3	1:B:538:PRO:HB3	1.99	0.44
1:D:618:PHE:HD1	1:D:618:PHE:C	2.25	0.44
1:G:265:ARG:HA	1:G:266:PRO:C	2.43	0.44
1:H:97:GLN:HG3	1:H:250:PHE:CD2	2.52	0.44
1:D:618:PHE:C	1:D:618:PHE:CD1	2.95	0.44
1:B:64:GLU:OE2	1:B:205:TYR:OH	2.24	0.44
1:G:603:ILE:O	1:G:607:GLU:HG3	2.18	0.44
1:H:389:LEU:HD23	1:H:389:LEU:C	2.42	0.44
1:A:158:THR:HG22	1:A:160:VAL:HG22	2.00	0.44
1:D:358:GLU:OE1	1:D:546:VAL:HG13	2.17	0.44
1:F:457:GLY:C	1:F:459:VAL:H	2.25	0.44
1:C:159:ARG:HA	2:C:801:FAD:O2B	2.17	0.44
1:D:319:THR:HG22	1:D:581:GLY:HA3	2.00	0.44
1:E:459:VAL:HG13	1:F:121:LEU:HB3	1.97	0.44
1:G:547:LEU:C	3:G:1101:HOH:O	2.61	0.44
1:B:121:LEU:HD21	1:C:121:LEU:HD23	1.99	0.44
1:E:104:VAL:CG2	1:E:453:ALA:C	2.91	0.44
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.83	0.44
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.83	0.43
1:A:104:VAL:CG2	1:A:453:ALA:C	2.91	0.43
1:F:515:ALA:HB3	1:G:128:PRO:HG2	2.00	0.43
1:A:105:ASN:O	1:B:105:ASN:HB3	2.19	0.43
1:A:495:TYR:O	1:A:496:ASN:CB	2.66	0.43
1:B:547:LEU:CD1	2:B:801:FAD:HM83	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:538:PRO:HG2	1:G:538:PRO:HG2	2.01	0.43
1:F:77:ILE:HD11	1:F:495:TYR:CD2	2.54	0.43
1:F:546:VAL:HG13	1:F:548:HIS:H	1.83	0.43
1:G:328:LEU:HD12	1:G:328:LEU:O	2.18	0.43
1:B:363:PHE:HA	1:B:471:TRP:O	2.19	0.43
1:F:158:THR:HG22	1:F:160:VAL:HG22	2.01	0.43
1:C:607:GLU:O	1:C:611:GLN:HG3	2.18	0.43
1:D:97:GLN:HG3	1:D:250:PHE:CD2	2.54	0.43
1:H:167:HIS:CD2	1:H:167:HIS:C	2.97	0.43
1:A:341:ASN:HD22	1:A:343:ALA:N	2.07	0.43
1:E:363:PHE:HA	1:E:471:TRP:O	2.19	0.43
1:E:380:MET:HE3	1:E:412:VAL:HB	2.00	0.43
1:E:167:HIS:NE2	2:E:801:FAD:HM81	2.10	0.42
1:E:381:THR:C	1:E:382:ILE:HD12	2.44	0.42
1:F:285:ARG:HA	1:F:328:LEU:HD13	1.99	0.42
1:F:167:HIS:CD2	1:F:167:HIS:C	2.96	0.42
1:H:97:GLN:HG3	1:H:250:PHE:CE2	2.54	0.42
1:B:47:TYR:O	1:B:313:ALA:HA	2.19	0.42
1:E:299:HIS:CA	1:E:310:GLU:OE1	2.68	0.42
1:A:82:SER:O	3:A:995:HOH:O	2.22	0.42
1:B:543:PRO:HG2	3:B:870:HOH:O	2.18	0.42
1:E:382:ILE:HD12	1:E:382:ILE:N	2.34	0.42
1:H:165:SER:HA	1:H:168:TRP:CD1	2.54	0.42
1:H:503:ASP:OD1	1:H:503:ASP:C	2.62	0.42
1:B:367:VAL:CG2	1:B:533:LEU:HD13	2.49	0.42
1:D:285:ARG:CA	1:D:328:LEU:HD11	2.49	0.42
1:F:385:THR:O	1:F:388:GLU:HB2	2.18	0.42
1:H:389:LEU:CD2	1:H:390:THR:HG23	2.50	0.42
1:A:104:VAL:HG22	1:A:453:ALA:HB1	2.01	0.42
1:H:471:TRP:CD1	1:H:471:TRP:N	2.87	0.42
1:A:548:HIS:HA	3:A:1057:HOH:O	2.19	0.42
1:C:132:GLN:CD	3:C:930:HOH:O	2.63	0.42
1:D:328:LEU:HD12	1:D:328:LEU:O	2.20	0.42
1:G:385:THR:O	1:G:391:TYR:HB2	2.19	0.42
1:H:215:GLU:O	1:H:411:LYS:NZ	2.53	0.42
1:H:457:GLY:O	1:H:461:GLN:HG3	2.20	0.42
1:G:389:LEU:N	1:G:389:LEU:CD1	2.83	0.42
1:H:513:LYS:NZ	1:H:517:ASP:OD2	2.50	0.42
1:A:126:LEU:HD13	1:A:132:GLN:CG	2.49	0.41
1:D:167:HIS:CD2	2:D:801:FAD:C8M	2.90	0.41
1:H:199:TYR:O	1:H:203:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:VAL:HG22	1:B:121:LEU:HD13	2.03	0.41
1:H:459:VAL:HG12	1:H:460:GLN:N	2.34	0.41
1:A:459:VAL:HA	1:A:462:SER:HB2	2.02	0.41
1:C:155:GLN:NE2	1:C:358:GLU:OE2	2.49	0.41
1:G:456:TYR:C	1:G:457:GLY:O	2.64	0.41
1:D:215:GLU:O	1:D:411:LYS:NZ	2.54	0.41
1:D:284:GLU:C	1:D:328:LEU:HD13	2.46	0.41
1:D:547:LEU:HD12	2:D:801:FAD:HM83	2.01	0.41
1:E:81:ASP:O	1:E:81:ASP:CG	2.62	0.41
1:F:155:GLN:NE2	1:F:358:GLU:OE2	2.50	0.41
1:F:167:HIS:NE2	2:F:801:FAD:HM81	2.14	0.41
1:G:81:ASP:OD1	1:G:81:ASP:C	2.63	0.41
1:H:44:ASP:HB3	1:H:46:LYS:H	1.85	0.41
1:A:206:PHE:CE2	1:A:599:MET:HE3	2.56	0.41
1:B:265:ARG:HA	1:B:266:PRO:C	2.46	0.41
1:F:439:PHE:CD1	1:F:439:PHE:C	2.99	0.41
1:H:459:VAL:HG12	1:H:460:GLN:HG3	2.01	0.41
1:C:383:ARG:HB2	1:C:392:SER:HB3	2.01	0.41
1:B:218:ARG:HD2	3:B:873:HOH:O	2.20	0.41
1:E:546:VAL:HG13	1:E:547:LEU:H	1.85	0.41
1:H:344:ASN:O	1:H:344:ASN:OD1	2.39	0.41
1:B:56:PRO:HD3	1:B:165:SER:HB3	2.03	0.41
1:B:359:GLN:NE2	1:B:591:GLY:O	2.54	0.41
1:E:167:HIS:NE2	2:E:801:FAD:C8	2.80	0.41
1:G:495:TYR:O	1:G:496:ASN:CB	2.69	0.41
1:F:546:VAL:CG1	1:F:547:LEU:N	2.83	0.41
1:G:105:ASN:O	1:H:105:ASN:HB3	2.21	0.41
1:C:326:THR:HG22	1:C:487:PHE:HE2	1.86	0.40
1:C:382:ILE:HD11	1:C:416:MET:HE1	2.02	0.40
1:D:43:MET:HE2	1:D:43:MET:HB3	1.99	0.40
1:G:167:HIS:CE1	2:G:801:FAD:C8M	2.90	0.40
1:B:167:HIS:CD2	2:B:801:FAD:C8	3.04	0.40
1:B:83:GLY:N	3:B:908:HOH:O	2.24	0.40
1:B:459:VAL:O	1:B:462:SER:CB	2.70	0.40
1:D:362:VAL:HG13	1:D:518:MET:HE3	2.04	0.40
1:E:159:ARG:HA	2:E:801:FAD:O2B	2.20	0.40
1:G:50:VAL:HG13	1:G:313:ALA:HB2	2.03	0.40
1:A:281:VAL:CG1	1:A:300:ILE:HB	2.51	0.40
1:C:105:ASN:HB3	1:D:105:ASN:O	2.22	0.40
1:C:285:ARG:HA	1:C:328:LEU:HD11	2.03	0.40
1:C:418:GLN:HE21	1:C:418:GLN:HB3	1.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:LEU:HD23	1:H:534:PRO:HD3	2.03	0.40
1:H:216:SER:HB3	1:H:219:HIS:HB3	2.04	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	575/623 (92%)	553 (96%)	22 (4%)	0	100	100
1	B	575/623 (92%)	556 (97%)	19 (3%)	0	100	100
1	C	575/623 (92%)	556 (97%)	19 (3%)	0	100	100
1	D	575/623 (92%)	557 (97%)	18 (3%)	0	100	100
1	E	575/623 (92%)	553 (96%)	21 (4%)	1 (0%)	43	44
1	F	575/623 (92%)	560 (97%)	15 (3%)	0	100	100
1	G	575/623 (92%)	552 (96%)	22 (4%)	1 (0%)	43	44
1	H	575/623 (92%)	555 (96%)	19 (3%)	1 (0%)	43	44
All	All	4600/4984 (92%)	4442 (97%)	155 (3%)	3 (0%)	48	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	344	ASN
1	E	187	ASP
1	G	457	GLY

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	504/541 (93%)	489 (97%)	15 (3%)	36	41
1	B	504/541 (93%)	486 (96%)	18 (4%)	31	34
1	C	504/541 (93%)	489 (97%)	15 (3%)	36	41
1	D	504/541 (93%)	493 (98%)	11 (2%)	45	53
1	E	504/541 (93%)	491 (97%)	13 (3%)	40	46
1	F	504/541 (93%)	486 (96%)	18 (4%)	31	34
1	G	504/541 (93%)	493 (98%)	11 (2%)	45	53
1	H	504/541 (93%)	489 (97%)	15 (3%)	36	41
All	All	4032/4328 (93%)	3916 (97%)	116 (3%)	37	42

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	121	LEU
1	A	185	LYS
1	A	206	PHE
1	A	312	LYS
1	A	328	LEU
1	A	341	ASN
1	A	388	GLU
1	A	394	THR
1	A	400	SER
1	A	401	THR
1	A	459	VAL
1	A	461	GLN
1	A	496	ASN
1	A	619	THR
1	B	44	ASP
1	B	45	ILE
1	B	95	GLU
1	B	100	ILE

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Mol	Chain	Res	Type
1	B	185	LYS
1	B	206	PHE
1	B	310	GLU
1	B	312	LYS
1	B	328	LEU
1	B	385	THR
1	B	389	LEU
1	B	408	TRP
1	B	421	GLU
1	B	455	SER
1	B	459	VAL
1	B	490	LYS
1	B	593	ASN
1	B	619	THR
1	C	45	ILE
1	C	104	VAL
1	C	185	LYS
1	C	336	GLN
1	C	344	ASN
1	C	385	THR
1	C	389	LEU
1	C	418	GLN
1	C	459	VAL
1	C	461	GLN
1	C	465	SER
1	C	490	LYS
1	C	496	ASN
1	C	576	LYS
1	C	619	THR
1	D	82	SER
1	D	100	ILE
1	D	104	VAL
1	D	194	GLU
1	D	206	PHE
1	D	328	LEU
1	D	385	THR
1	D	388	GLU
1	D	389	LEU
1	D	459	VAL
1	D	560	LYS
1	E	44	ASP
1	E	45	ILE

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Mol	Chain	Res	Type
1	E	185	LYS
1	E	206	PHE
1	E	228	GLU
1	E	231	LYS
1	E	312	LYS
1	E	328	LEU
1	E	385	THR
1	E	388	GLU
1	E	403	LYS
1	E	459	VAL
1	E	490	LYS
1	F	121	LEU
1	F	178	GLU
1	F	206	PHE
1	F	228	GLU
1	F	328	LEU
1	F	336	GLN
1	F	344	ASN
1	F	385	THR
1	F	392	SER
1	F	400	SER
1	F	421	GLU
1	F	459	VAL
1	F	460	GLN
1	F	461	GLN
1	F	465	SER
1	F	490	LYS
1	F	546	VAL
1	F	576	LYS
1	G	45	ILE
1	G	100	ILE
1	G	104	VAL
1	G	228	GLU
1	G	272	GLU
1	G	385	THR
1	G	389	LEU
1	G	408	TRP
1	G	459	VAL
1	G	490	LYS
1	G	496	ASN
1	H	45	ILE
1	H	100	ILE

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Mol	Chain	Res	Type
1	H	104	VAL
1	H	132	GLN
1	H	185	LYS
1	H	206	PHE
1	H	328	LEU
1	H	389	LEU
1	H	400	SER
1	H	455	SER
1	H	459	VAL
1	H	460	GLN
1	H	496	ASN
1	H	546	VAL
1	H	593	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	263	GLN
1	A	324	HIS
1	A	341	ASN
1	A	419	HIS
1	A	440	GLN
1	A	499	GLN
1	B	233	GLN
1	B	257	ASN
1	B	263	GLN
1	B	336	GLN
1	B	611	GLN
1	C	105	ASN
1	C	108	GLN
1	C	132	GLN
1	C	263	GLN
1	C	276	ASN
1	C	299	HIS
1	C	324	HIS
1	C	341	ASN
1	C	344	ASN
1	C	418	GLN
1	C	448	GLN
1	C	499	GLN
1	D	220	ASN

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Mol	Chain	Res	Type
1	D	257	ASN
1	D	263	GLN
1	D	299	HIS
1	D	324	HIS
1	D	336	GLN
1	D	460	GLN
1	E	99	ASN
1	E	233	GLN
1	E	257	ASN
1	E	263	GLN
1	E	418	GLN
1	E	460	GLN
1	E	611	GLN
1	F	99	ASN
1	F	263	GLN
1	F	299	HIS
1	F	301	HIS
1	F	324	HIS
1	F	419	HIS
1	F	593	ASN
1	G	108	GLN
1	G	233	GLN
1	G	257	ASN
1	G	263	GLN
1	G	324	HIS
1	G	418	GLN
1	G	460	GLN
1	G	461	GLN
1	H	105	ASN
1	H	110	GLN
1	H	132	GLN
1	H	257	ASN
1	H	263	GLN
1	H	324	HIS
1	H	341	ASN
1	H	419	HIS
1	H	440	GLN
1	H	460	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	G	801	1	58,58,58	1.54	11 (18%)	85,89,89	2.68	37 (43%)
2	FAD	C	801	1	58,58,58	1.54	10 (17%)	85,89,89	2.75	35 (41%)
2	FAD	F	801	1	58,58,58	1.40	9 (15%)	85,89,89	2.57	30 (35%)
2	FAD	H	801	1	58,58,58	1.47	8 (13%)	85,89,89	2.52	35 (41%)
2	FAD	D	801	1	58,58,58	1.65	13 (22%)	85,89,89	2.55	33 (38%)
2	FAD	E	801	1	58,58,58	1.39	6 (10%)	85,89,89	2.50	31 (36%)
2	FAD	B	801	1	58,58,58	1.65	11 (18%)	85,89,89	2.44	31 (36%)
2	FAD	A	801	1	58,58,58	1.54	12 (20%)	85,89,89	2.59	32 (37%)

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	G	801	1	-	1/34/50/50	0/6/6/6
2	FAD	C	801	1	-	1/34/50/50	0/6/6/6
2	FAD	F	801	1	-	3/34/50/50	0/6/6/6
2	FAD	H	801	1	-	1/34/50/50	0/6/6/6
2	FAD	D	801	1	-	4/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	E	801	1	-	3/34/50/50	0/6/6/6
2	FAD	B	801	1	-	1/34/50/50	0/6/6/6
2	FAD	A	801	1	-	0/34/50/50	0/6/6/6

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	FAD	PA-O3P	7.27	1.67	1.59
2	C	801	FAD	P-O3P	4.95	1.64	1.59
2	E	801	FAD	P-O3P	4.77	1.64	1.59
2	B	801	FAD	PA-O3P	4.70	1.64	1.59
2	H	801	FAD	C6-C5X	4.53	1.46	1.40
2	H	801	FAD	PA-O3P	4.02	1.63	1.59
2	B	801	FAD	C8A-N9A	-3.84	1.31	1.37
2	H	801	FAD	P-O3P	3.80	1.63	1.59
2	F	801	FAD	C4X-N5	3.77	1.38	1.30
2	G	801	FAD	P-O3P	3.76	1.63	1.59
2	C	801	FAD	C6-C5X	3.74	1.45	1.40
2	D	801	FAD	P-O3P	3.56	1.63	1.59
2	G	801	FAD	C10-N1	3.53	1.40	1.33
2	B	801	FAD	C6-C5X	3.46	1.45	1.40
2	A	801	FAD	P-O3P	3.45	1.63	1.59
2	E	801	FAD	PA-O3P	3.40	1.63	1.59
2	A	801	FAD	C2B-C3B	-3.36	1.44	1.53
2	A	801	FAD	C2-N3	-3.34	1.31	1.39
2	A	801	FAD	O2B-C2B	-3.29	1.34	1.43
2	C	801	FAD	C8A-N9A	-3.27	1.32	1.37
2	B	801	FAD	C5X-N5	-3.16	1.33	1.39
2	B	801	FAD	C4A-N9A	-3.12	1.31	1.37
2	G	801	FAD	O2B-C2B	-3.10	1.35	1.43
2	G	801	FAD	PA-O3P	3.05	1.62	1.59
2	B	801	FAD	C7M-C7	2.98	1.56	1.51
2	B	801	FAD	C2B-C3B	-2.97	1.45	1.53
2	A	801	FAD	C8A-N9A	-2.92	1.32	1.37
2	H	801	FAD	C5A-N7A	-2.89	1.33	1.39
2	D	801	FAD	C8A-N9A	-2.89	1.32	1.37
2	G	801	FAD	O4B-C4B	-2.86	1.38	1.45
2	E	801	FAD	C5A-N7A	-2.85	1.33	1.39
2	B	801	FAD	C2-N3	-2.80	1.32	1.39
2	G	801	FAD	C2-N3	-2.78	1.32	1.39
2	F	801	FAD	C1'-C2'	-2.73	1.48	1.52
2	A	801	FAD	C4-N3	-2.73	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	FAD	C5A-N7A	-2.64	1.34	1.39
2	C	801	FAD	C10-N1	2.63	1.38	1.33
2	C	801	FAD	O3B-C3B	-2.60	1.36	1.43
2	F	801	FAD	C6-C5X	2.60	1.43	1.40
2	F	801	FAD	C4-N3	-2.57	1.34	1.38
2	H	801	FAD	C2-N3	-2.54	1.33	1.39
2	F	801	FAD	O2B-C2B	-2.53	1.36	1.43
2	F	801	FAD	C2-N3	-2.52	1.33	1.39
2	C	801	FAD	C8A-N7A	2.49	1.36	1.31
2	B	801	FAD	O2B-C2B	-2.46	1.36	1.43
2	D	801	FAD	C6-C5X	2.43	1.43	1.40
2	G	801	FAD	C8A-N9A	-2.43	1.33	1.37
2	H	801	FAD	C8A-N9A	-2.42	1.33	1.37
2	B	801	FAD	C4-N3	-2.40	1.34	1.38
2	A	801	FAD	O2'-C2'	-2.40	1.38	1.43
2	G	801	FAD	C2B-C3B	-2.37	1.46	1.53
2	C	801	FAD	C4X-N5	2.32	1.35	1.30
2	A	801	FAD	C5A-N7A	-2.32	1.34	1.39
2	A	801	FAD	C4'-C3'	-2.31	1.49	1.53
2	C	801	FAD	C2-N3	-2.29	1.34	1.39
2	D	801	FAD	C9A-C5X	-2.28	1.37	1.41
2	F	801	FAD	C4X-C10	-2.28	1.37	1.44
2	D	801	FAD	C5X-N5	-2.23	1.35	1.39
2	D	801	FAD	C3B-C4B	-2.21	1.47	1.53
2	G	801	FAD	C7M-C7	2.20	1.55	1.51
2	E	801	FAD	C5X-N5	-2.20	1.35	1.39
2	A	801	FAD	C4A-N9A	-2.19	1.33	1.37
2	G	801	FAD	O3B-C3B	-2.17	1.37	1.43
2	C	801	FAD	C5X-N5	-2.17	1.35	1.39
2	E	801	FAD	O4'-C4'	-2.14	1.38	1.43
2	D	801	FAD	C5A-N7A	-2.13	1.35	1.39
2	G	801	FAD	C4X-C10	-2.12	1.37	1.44
2	D	801	FAD	C2-N3	-2.12	1.34	1.39
2	D	801	FAD	PA-O2A	-2.12	1.45	1.55
2	B	801	FAD	P-O3P	2.11	1.61	1.59
2	E	801	FAD	C4'-C3'	-2.09	1.49	1.53
2	D	801	FAD	O3B-C3B	-2.08	1.37	1.43
2	D	801	FAD	O5B-C5B	-2.07	1.36	1.44
2	A	801	FAD	C4X-C10	-2.07	1.38	1.44
2	H	801	FAD	C2-N1	-2.06	1.32	1.36
2	H	801	FAD	C2A-N1A	2.04	1.37	1.33
2	D	801	FAD	C2B-C3B	-2.04	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FAD	C2A-N1A	2.03	1.37	1.33
2	F	801	FAD	O2'-C2'	-2.02	1.39	1.43
2	A	801	FAD	C8M-C8	-2.00	1.47	1.51

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	C4A-N9A-C8A	8.83	115.01	105.74
2	A	801	FAD	C4A-N9A-C8A	7.80	113.93	105.74
2	H	801	FAD	C4A-N9A-C8A	7.69	113.81	105.74
2	A	801	FAD	C4-N3-C2	7.68	139.28	125.64
2	F	801	FAD	N3A-C2A-N1A	-7.46	117.29	128.58
2	C	801	FAD	C4A-N9A-C8A	7.39	113.49	105.74
2	A	801	FAD	N9A-C8A-N7A	-7.08	103.89	113.94
2	G	801	FAD	C4A-N9A-C8A	6.97	113.06	105.74
2	A	801	FAD	N3A-C2A-N1A	-6.78	118.32	128.58
2	G	801	FAD	N3A-C2A-N1A	-6.64	118.52	128.58
2	C	801	FAD	O4B-C1B-N9A	6.62	120.81	108.09
2	D	801	FAD	O4B-C1B-N9A	6.55	120.68	108.09
2	C	801	FAD	N3A-C2A-N1A	-6.55	118.66	128.58
2	C	801	FAD	C4-C4X-N5	6.46	127.13	118.21
2	B	801	FAD	N9A-C8A-N7A	-6.40	104.85	113.94
2	H	801	FAD	N3A-C2A-N1A	-6.39	118.90	128.58
2	F	801	FAD	C4A-N9A-C8A	6.36	112.41	105.74
2	D	801	FAD	C4A-N9A-C8A	6.16	112.21	105.74
2	A	801	FAD	O3B-C3B-C4B	6.07	128.53	111.08
2	H	801	FAD	N9A-C8A-N7A	-6.05	105.35	113.94
2	E	801	FAD	C4A-N9A-C8A	5.90	111.94	105.74
2	F	801	FAD	O4B-C1B-N9A	5.90	119.42	108.09
2	C	801	FAD	N9A-C8A-N7A	-5.89	105.58	113.94
2	F	801	FAD	C2B-C1B-N9A	5.87	127.88	113.30
2	G	801	FAD	N3-C2-N1	-5.85	107.07	119.50
2	E	801	FAD	O4-C4-N3	5.84	131.09	120.11
2	D	801	FAD	N3A-C2A-N1A	-5.83	119.76	128.58
2	E	801	FAD	N3A-C2A-N1A	-5.73	119.91	128.58
2	G	801	FAD	C4-C4X-C10	-5.73	107.11	116.93
2	C	801	FAD	O4-C4-C4X	-5.71	111.44	126.53
2	H	801	FAD	C2B-C1B-N9A	5.70	127.47	113.30
2	G	801	FAD	N9A-C8A-N7A	-5.65	105.92	113.94
2	D	801	FAD	C9A-C5X-N5	-5.64	116.47	122.45
2	G	801	FAD	O3B-C3B-C4B	5.63	127.25	111.08
2	E	801	FAD	N9A-C8A-N7A	-5.58	106.01	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	FAD	C1B-N9A-C8A	-5.56	114.76	127.09
2	H	801	FAD	O3B-C3B-C4B	5.49	126.84	111.08
2	F	801	FAD	N9A-C8A-N7A	-5.41	106.26	113.94
2	E	801	FAD	O4B-C1B-N9A	5.40	118.46	108.09
2	E	801	FAD	C2B-C1B-N9A	5.28	126.43	113.30
2	C	801	FAD	O3B-C3B-C4B	5.24	126.12	111.08
2	D	801	FAD	N9A-C8A-N7A	-5.22	106.53	113.94
2	F	801	FAD	C2A-N1A-C6A	5.17	127.23	118.73
2	F	801	FAD	O4-C4-C4X	-5.12	113.01	126.53
2	G	801	FAD	O4B-C1B-N9A	5.11	117.90	108.09
2	E	801	FAD	O2B-C2B-C3B	5.08	128.12	111.82
2	C	801	FAD	O2B-C2B-C1B	5.08	127.59	110.10
2	E	801	FAD	O3B-C3B-C4B	5.06	125.63	111.08
2	C	801	FAD	C2B-C1B-N9A	5.05	125.86	113.30
2	B	801	FAD	O4-C4-N3	5.04	129.60	120.11
2	B	801	FAD	N3A-C2A-N1A	-4.98	121.04	128.58
2	B	801	FAD	C2B-C1B-N9A	4.98	125.67	113.30
2	F	801	FAD	O4-C4-N3	4.96	129.43	120.11
2	G	801	FAD	C2B-C1B-N9A	4.93	125.56	113.30
2	E	801	FAD	O4-C4-C4X	-4.86	113.72	126.53
2	C	801	FAD	C9A-C5X-N5	-4.80	117.36	122.45
2	H	801	FAD	N3A-C4A-N9A	4.78	135.30	127.17
2	D	801	FAD	O3B-C3B-C4B	4.74	124.69	111.08
2	F	801	FAD	C9A-C5X-N5	-4.72	117.44	122.45
2	D	801	FAD	O4-C4-N3	4.71	128.97	120.11
2	B	801	FAD	O4-C4-C4X	-4.66	114.24	126.53
2	F	801	FAD	N3A-C4A-N9A	4.65	135.08	127.17
2	D	801	FAD	C2B-C1B-N9A	4.59	124.71	113.30
2	A	801	FAD	C4X-C4-N3	-4.58	101.59	113.25
2	C	801	FAD	O4-C4-N3	4.57	128.71	120.11
2	C	801	FAD	N3A-C4A-N9A	4.53	134.88	127.17
2	A	801	FAD	C2B-C1B-N9A	4.49	124.46	113.30
2	H	801	FAD	O2B-C2B-C1B	4.47	125.50	110.10
2	A	801	FAD	N3-C2-N1	-4.47	110.01	119.50
2	G	801	FAD	O4-C4-C4X	-4.45	114.78	126.53
2	H	801	FAD	C9A-C5X-N5	-4.40	117.79	122.45
2	F	801	FAD	O3B-C3B-C4B	4.37	123.64	111.08
2	D	801	FAD	C5A-N7A-C8A	4.33	110.25	103.45
2	H	801	FAD	C4-N3-C2	4.31	133.30	125.64
2	E	801	FAD	C9A-C5X-N5	-4.30	117.89	122.45
2	E	801	FAD	O2B-C2B-C1B	4.30	124.92	110.10
2	C	801	FAD	C5A-C4A-N3A	-4.15	121.00	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	FAD	C4-N3-C2	4.15	133.02	125.64
2	A	801	FAD	C5A-N7A-C8A	4.13	109.94	103.45
2	A	801	FAD	O4B-C4B-C5B	4.13	122.55	109.33
2	E	801	FAD	C5B-C4B-C3B	4.12	130.06	115.21
2	B	801	FAD	O2B-C2B-C1B	4.10	124.23	110.10
2	D	801	FAD	O2B-C2B-C1B	4.08	124.17	110.10
2	D	801	FAD	C1B-N9A-C8A	-4.06	118.09	127.09
2	D	801	FAD	C2A-N1A-C6A	4.01	125.31	118.73
2	B	801	FAD	C5A-N7A-C8A	3.97	109.68	103.45
2	F	801	FAD	C1B-N9A-C8A	-3.95	118.34	127.09
2	E	801	FAD	C5A-N7A-C8A	3.92	109.62	103.45
2	C	801	FAD	C9-C8-C7	3.91	125.42	119.69
2	D	801	FAD	N3A-C4A-N9A	3.90	133.81	127.17
2	B	801	FAD	O4B-C4B-C5B	3.90	121.83	109.33
2	G	801	FAD	C10-N1-C2	3.90	125.29	116.85
2	E	801	FAD	N3A-C4A-N9A	3.88	133.77	127.17
2	G	801	FAD	C2A-N1A-C6A	3.88	125.10	118.73
2	F	801	FAD	C9-C8-C7	3.86	125.35	119.69
2	G	801	FAD	N3A-C4A-N9A	3.85	133.71	127.17
2	G	801	FAD	O2-C2-N3	3.84	125.95	118.58
2	G	801	FAD	C5A-N7A-C8A	3.81	109.43	103.45
2	H	801	FAD	O2B-C2B-C3B	3.80	124.01	111.82
2	F	801	FAD	C4-N3-C2	3.65	132.13	125.64
2	C	801	FAD	C2A-N3A-C4A	3.60	120.63	111.83
2	H	801	FAD	O4B-C1B-C2B	3.59	114.30	106.62
2	B	801	FAD	C8M-C8-C9	-3.59	113.25	119.57
2	C	801	FAD	C5A-N7A-C8A	3.58	109.08	103.45
2	B	801	FAD	O4B-C1B-N9A	3.57	114.95	108.09
2	E	801	FAD	C2A-N1A-C6A	3.56	124.58	118.73
2	C	801	FAD	O2B-C2B-C3B	3.50	123.03	111.82
2	A	801	FAD	C9A-C5X-N5	-3.49	118.75	122.45
2	D	801	FAD	C4-C4X-C10	3.44	122.83	116.93
2	B	801	FAD	C5X-C6-C7	-3.44	114.46	120.83
2	A	801	FAD	C2A-N1A-C6A	3.42	124.35	118.73
2	A	801	FAD	O4B-C4B-C3B	3.41	111.93	105.15
2	H	801	FAD	O4B-C1B-N9A	3.40	114.62	108.09
2	H	801	FAD	C1B-N9A-C8A	-3.40	119.56	127.09
2	D	801	FAD	C5A-C4A-N3A	-3.39	122.05	126.72
2	F	801	FAD	O3P-PA-O1A	-3.39	100.51	110.70
2	D	801	FAD	C10-C4X-N5	-3.36	117.95	124.81
2	A	801	FAD	C2A-N3A-C4A	3.36	120.03	111.83
2	G	801	FAD	O3P-PA-O1A	-3.34	100.64	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	C1B-N9A-C8A	-3.33	119.71	127.09
2	B	801	FAD	C9A-C5X-N5	-3.32	118.93	122.45
2	H	801	FAD	C5A-C4A-N3A	-3.30	122.17	126.72
2	F	801	FAD	C5A-C4A-N3A	-3.29	122.19	126.72
2	A	801	FAD	O2B-C2B-C1B	3.29	121.42	110.10
2	C	801	FAD	C5B-C4B-C3B	3.28	127.03	115.21
2	A	801	FAD	C4-C4X-C10	3.26	122.52	116.93
2	D	801	FAD	C4A-C5A-N7A	-3.23	106.89	110.58
2	D	801	FAD	O4B-C4B-C5B	3.23	119.67	109.33
2	H	801	FAD	C5A-C4A-N9A	-3.22	102.30	105.81
2	D	801	FAD	O2A-PA-O3P	3.20	115.91	107.27
2	G	801	FAD	C2A-N3A-C4A	3.16	119.56	111.83
2	B	801	FAD	N3A-C4A-N9A	3.15	132.53	127.17
2	B	801	FAD	C2A-N1A-C6A	3.15	123.91	118.73
2	H	801	FAD	O4B-C4B-C3B	3.15	111.41	105.15
2	A	801	FAD	O3P-PA-O1A	-3.15	101.24	110.70
2	H	801	FAD	C5A-N7A-C8A	3.14	108.39	103.45
2	H	801	FAD	C8M-C8-C9	-3.13	114.06	119.57
2	G	801	FAD	O4B-C4B-C5B	3.12	119.32	109.33
2	C	801	FAD	C5'-C4'-C3'	-3.12	106.34	112.22
2	G	801	FAD	O2B-C2B-C3B	3.10	121.76	111.82
2	E	801	FAD	O3P-PA-O1A	-3.09	101.41	110.70
2	A	801	FAD	C4B-O4B-C1B	-3.08	102.66	109.47
2	B	801	FAD	C4A-C5A-N7A	-3.08	107.06	110.58
2	H	801	FAD	C2A-N3A-C4A	3.05	119.27	111.83
2	C	801	FAD	O3P-PA-O1A	-3.03	101.59	110.70
2	F	801	FAD	C2A-N3A-C4A	3.01	119.18	111.83
2	G	801	FAD	C8M-C8-C9	-3.00	114.28	119.57
2	F	801	FAD	C5X-C9A-N10	3.00	120.68	117.97
2	F	801	FAD	C5A-N7A-C8A	2.99	108.14	103.45
2	D	801	FAD	O4B-C4B-C3B	2.98	111.07	105.15
2	F	801	FAD	O2B-C2B-C1B	2.97	120.33	110.10
2	E	801	FAD	C1B-N9A-C8A	-2.96	120.52	127.09
2	A	801	FAD	O4B-C1B-C2B	2.96	112.94	106.62
2	B	801	FAD	O3B-C3B-C4B	2.95	119.57	111.08
2	B	801	FAD	C9-C8-C7	2.95	124.01	119.69
2	G	801	FAD	C5A-C4A-N3A	-2.94	122.66	126.72
2	F	801	FAD	O2B-C2B-C3B	2.94	121.24	111.82
2	F	801	FAD	C5A-C4A-N9A	-2.90	102.65	105.81
2	H	801	FAD	O4'-C4'-C3'	2.89	116.00	109.25
2	F	801	FAD	C5B-C4B-C3B	2.87	125.54	115.21
2	E	801	FAD	C5A-C4A-N3A	-2.84	122.81	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O3'-C3'-C2'	-2.83	102.50	108.93
2	D	801	FAD	C4-N3-C2	2.80	130.62	125.64
2	D	801	FAD	O2B-C2B-C3B	2.79	120.77	111.82
2	B	801	FAD	O3P-PA-O1A	-2.79	102.33	110.70
2	A	801	FAD	N3A-C4A-N9A	2.76	131.86	127.17
2	G	801	FAD	O2B-C2B-C1B	2.74	119.53	110.10
2	A	801	FAD	O2B-C2B-C3B	2.73	120.57	111.82
2	C	801	FAD	O2A-PA-O1A	2.72	125.08	112.44
2	E	801	FAD	C5X-C9A-N10	2.71	120.42	117.97
2	E	801	FAD	O2P-P-O3P	-2.71	99.95	107.27
2	A	801	FAD	O3P-P-O1P	2.70	118.82	110.70
2	C	801	FAD	C4A-C5A-N7A	-2.70	107.50	110.58
2	H	801	FAD	C4B-O4B-C1B	-2.69	103.53	109.47
2	E	801	FAD	O2A-PA-O3P	2.67	114.50	107.27
2	H	801	FAD	O4-C4-N3	2.64	125.08	120.11
2	E	801	FAD	C5'-C4'-C3'	-2.64	107.23	112.22
2	B	801	FAD	C10-C4X-N5	-2.64	119.43	124.81
2	C	801	FAD	C5X-N5-C4X	2.62	122.33	118.09
2	E	801	FAD	O4B-C4B-C3B	2.61	110.34	105.15
2	H	801	FAD	C2A-N1A-C6A	2.60	123.01	118.73
2	D	801	FAD	C2A-N3A-C4A	2.60	118.18	111.83
2	H	801	FAD	O2A-PA-O1A	2.59	124.48	112.44
2	E	801	FAD	O2A-PA-O1A	2.58	124.43	112.44
2	G	801	FAD	C5B-C4B-C3B	2.57	124.46	115.21
2	B	801	FAD	O2A-PA-O3P	2.56	114.18	107.27
2	F	801	FAD	O2A-PA-O3P	2.55	114.17	107.27
2	B	801	FAD	O3P-P-O1P	2.55	118.38	110.70
2	D	801	FAD	O2P-P-O1P	2.54	124.28	112.44
2	B	801	FAD	C4-C4X-N5	2.52	121.68	118.21
2	C	801	FAD	C4-C4X-C10	-2.51	112.62	116.93
2	G	801	FAD	C4A-C5A-N7A	-2.47	107.76	110.58
2	G	801	FAD	C5X-C6-C7	-2.46	116.27	120.83
2	C	801	FAD	C2A-N1A-C6A	2.45	122.76	118.73
2	F	801	FAD	O2A-PA-O1A	2.45	123.84	112.44
2	H	801	FAD	O4B-C4B-C5B	2.45	117.17	109.33
2	E	801	FAD	O3B-C3B-C2B	2.43	119.61	111.82
2	D	801	FAD	C7M-C7-C6	2.43	123.85	119.57
2	H	801	FAD	C5B-C4B-C3B	2.42	123.93	115.21
2	H	801	FAD	C5'-C4'-C3'	-2.42	107.65	112.22
2	H	801	FAD	O2P-P-O3P	-2.42	100.74	107.27
2	H	801	FAD	C4'-C3'-C2'	-2.42	109.55	113.57
2	G	801	FAD	C4-C4X-N5	2.41	121.54	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	C4A-C5A-N7A	-2.40	107.84	110.58
2	A	801	FAD	C5A-C4A-N3A	-2.39	123.42	126.72
2	G	801	FAD	C5A-C6A-N6A	2.39	129.21	123.29
2	C	801	FAD	N3-C2-N1	-2.39	114.43	119.50
2	C	801	FAD	C4-N3-C2	2.38	129.88	125.64
2	D	801	FAD	C4X-C4-N3	-2.36	107.24	113.25
2	E	801	FAD	C2A-N3A-C4A	2.33	117.53	111.83
2	C	801	FAD	C8M-C8-C9	-2.32	115.48	119.57
2	B	801	FAD	C8M-C8-C7	-2.32	116.02	120.76
2	B	801	FAD	O2P-P-O3P	-2.32	101.00	107.27
2	H	801	FAD	O2-C2-N3	2.32	123.03	118.58
2	B	801	FAD	C5A-C4A-N9A	-2.29	103.31	105.81
2	A	801	FAD	C1B-N9A-C8A	-2.28	122.03	127.09
2	B	801	FAD	O4B-C1B-C2B	2.27	111.48	106.62
2	D	801	FAD	O3P-PA-O1A	-2.27	103.88	110.70
2	G	801	FAD	O2A-PA-O3P	2.27	113.40	107.27
2	C	801	FAD	O4'-C4'-C3'	2.26	114.54	109.25
2	C	801	FAD	C10-C4X-N5	-2.26	120.20	124.81
2	B	801	FAD	C5B-C4B-C3B	2.25	123.32	115.21
2	A	801	FAD	O2-C2-N3	2.25	122.90	118.58
2	E	801	FAD	C8M-C8-C7	-2.25	116.16	120.76
2	H	801	FAD	C9-C8-C7	2.24	122.97	119.69
2	E	801	FAD	C6-C5X-C9A	-2.24	115.98	119.05
2	E	801	FAD	C5A-C4A-N9A	-2.22	103.40	105.81
2	C	801	FAD	C6-C5X-C9A	2.21	122.09	119.05
2	A	801	FAD	C5X-N5-C4X	2.21	121.66	118.09
2	D	801	FAD	C5X-N5-C4X	2.20	121.65	118.09
2	F	801	FAD	N3-C2-N1	-2.20	114.83	119.50
2	H	801	FAD	O3P-PA-O1A	-2.18	104.14	110.70
2	A	801	FAD	C10-N1-C2	2.17	121.54	116.85
2	H	801	FAD	O3P-P-O1P	2.16	117.21	110.70
2	D	801	FAD	C8M-C8-C9	-2.16	115.77	119.57
2	D	801	FAD	O5'-P-O1P	-2.16	100.39	108.94
2	G	801	FAD	C4'-C3'-C2'	-2.16	109.98	113.57
2	D	801	FAD	C5A-C6A-N6A	2.15	128.62	123.29
2	F	801	FAD	O3B-C3B-C2B	2.14	118.69	111.82
2	C	801	FAD	C5X-C6-C7	-2.14	116.86	120.83
2	E	801	FAD	O2P-P-O1P	2.14	122.39	112.44
2	B	801	FAD	O2'-C2'-C3'	2.13	114.24	109.25
2	G	801	FAD	C5X-N5-C4X	2.13	121.53	118.09
2	H	801	FAD	C5X-C9A-N10	2.13	119.89	117.97
2	G	801	FAD	C9A-C5X-N5	-2.13	120.20	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O2P-P-O3P	-2.12	101.54	107.27
2	G	801	FAD	C7M-C7-C6	-2.12	115.84	119.57
2	G	801	FAD	O4'-C4'-C3'	2.11	114.18	109.25
2	A	801	FAD	C9-C8-C7	2.11	122.78	119.69
2	G	801	FAD	O4B-C4B-C3B	2.10	109.33	105.15
2	H	801	FAD	C2'-C1'-N10	2.10	120.14	110.20
2	G	801	FAD	C4A-N9A-C1B	2.10	131.53	126.63
2	E	801	FAD	O5B-C5B-C4B	2.08	116.07	108.99
2	C	801	FAD	C9A-C9-C8	-2.07	115.06	119.22
2	B	801	FAD	C5X-C9A-N10	2.07	119.84	117.97
2	G	801	FAD	C5A-C4A-N9A	-2.07	103.56	105.81
2	B	801	FAD	O2B-C2B-C3B	2.07	118.45	111.82
2	C	801	FAD	O4B-C4B-C5B	2.05	115.90	109.33
2	A	801	FAD	C5X-C6-C7	-2.05	117.03	120.83
2	F	801	FAD	C6-C5X-N5	2.04	121.84	118.44
2	F	801	FAD	C8M-C8-C9	-2.04	115.97	119.57
2	A	801	FAD	O5'-P-O1P	-2.03	100.89	108.94
2	A	801	FAD	C3B-C2B-C1B	2.02	105.28	101.46
2	F	801	FAD	C9-C9A-N10	-2.01	119.15	121.85

There are no chirality outliers.

All (14) torsion outliers are listed below:

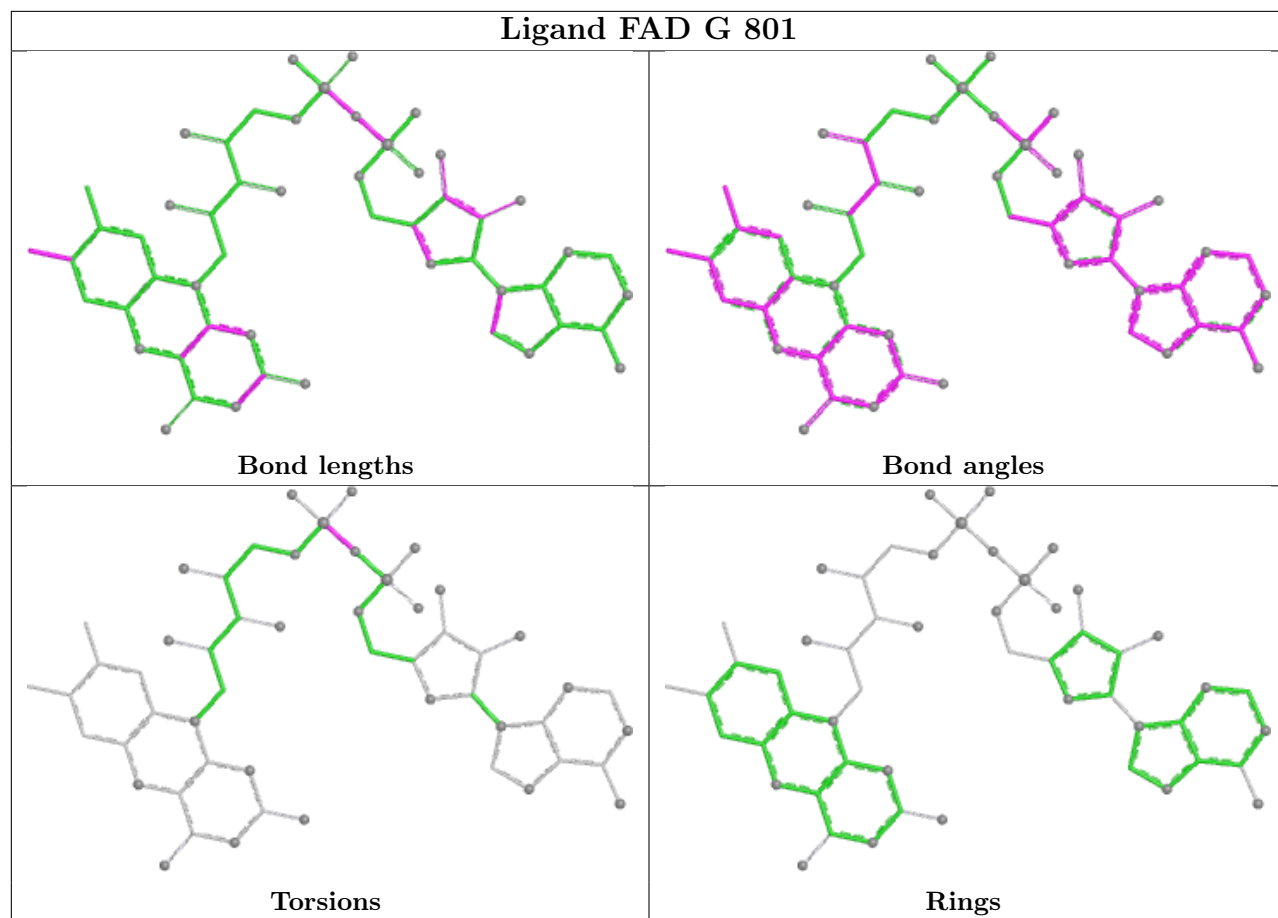
Mol	Chain	Res	Type	Atoms
2	E	801	FAD	PA-O3P-P-O5'
2	B	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
2	F	801	FAD	PA-O3P-P-O5'
2	G	801	FAD	PA-O3P-P-O5'
2	C	801	FAD	O4B-C4B-C5B-O5B
2	E	801	FAD	C3B-C4B-C5B-O5B
2	F	801	FAD	O4B-C4B-C5B-O5B
2	E	801	FAD	P-O3P-PA-O2A
2	H	801	FAD	PA-O3P-P-O5'
2	F	801	FAD	P-O3P-PA-O2A
2	D	801	FAD	O4B-C1B-N9A-C8A
2	D	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	P-O3P-PA-O2A

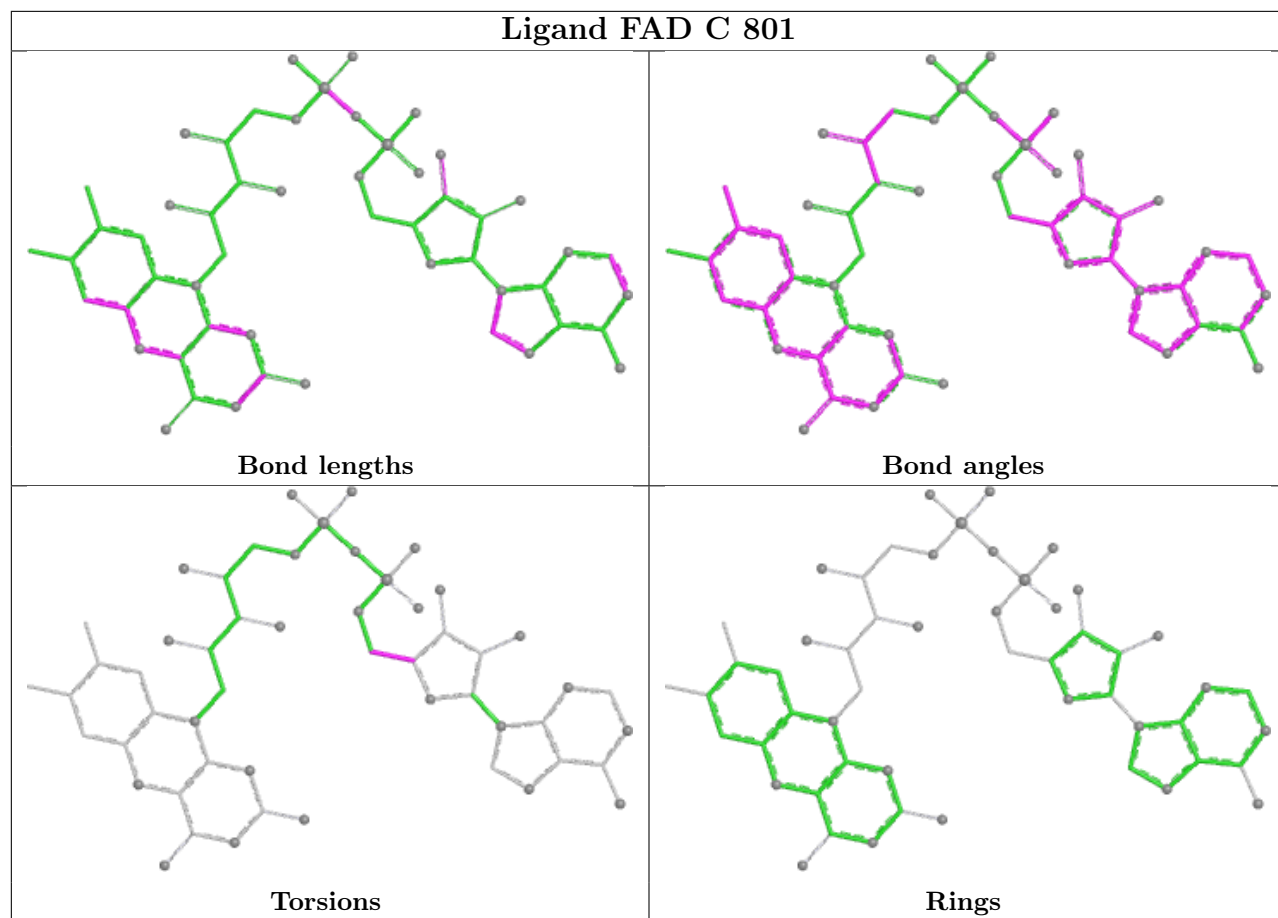
There are no ring outliers.

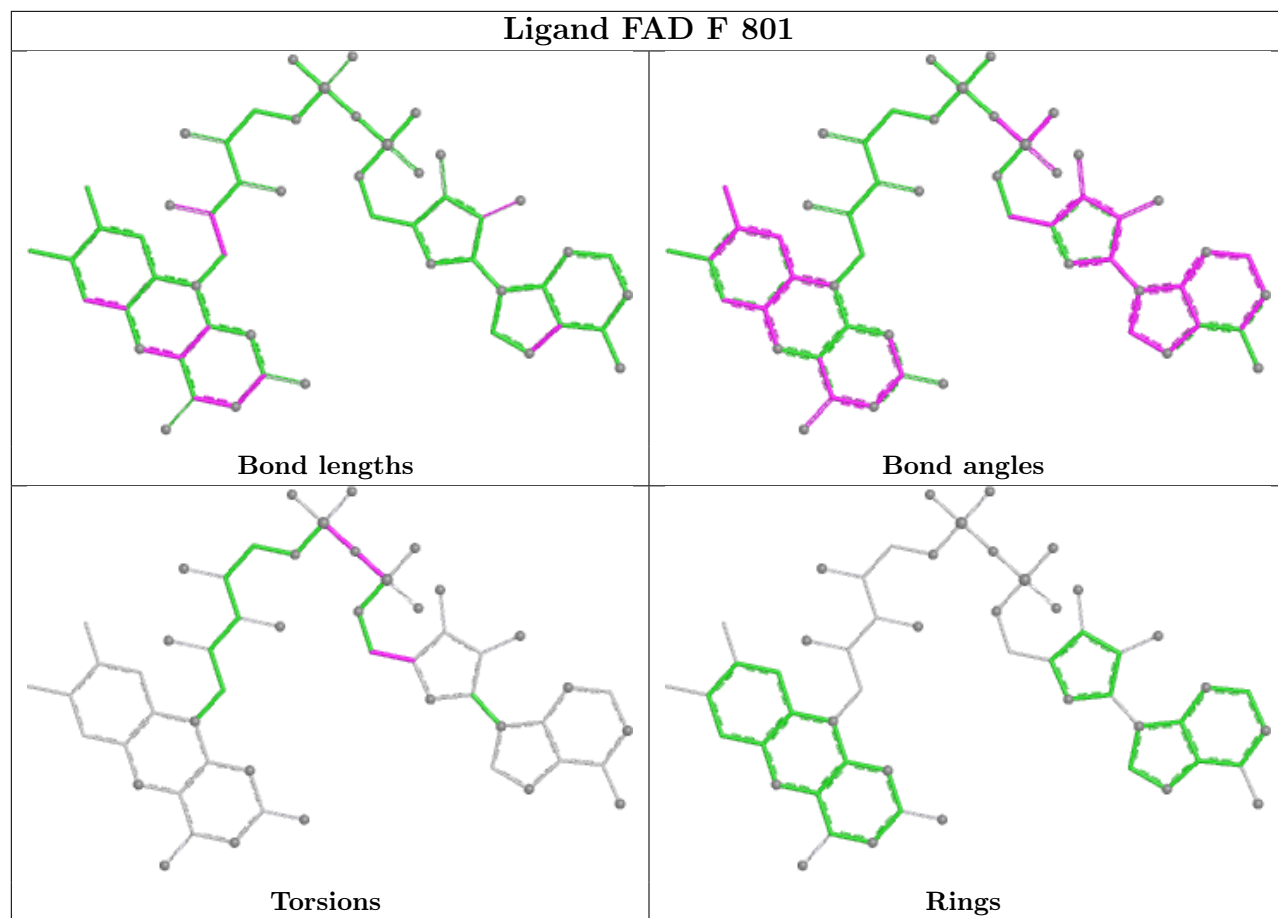
8 monomers are involved in 60 short contacts:

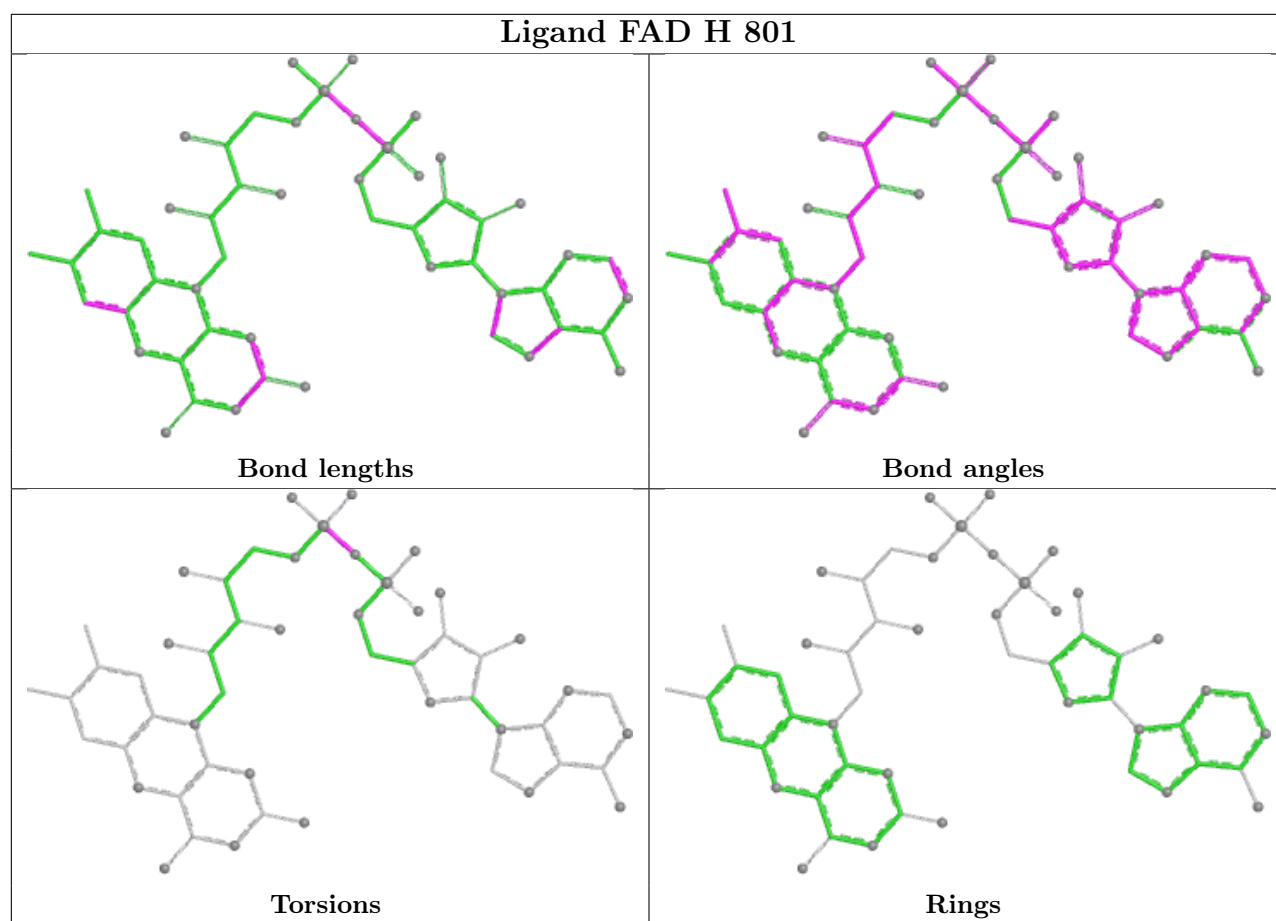
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	801	FAD	9	0
2	C	801	FAD	5	0
2	F	801	FAD	5	0
2	H	801	FAD	5	0
2	D	801	FAD	8	0
2	E	801	FAD	8	0
2	B	801	FAD	14	0
2	A	801	FAD	6	0

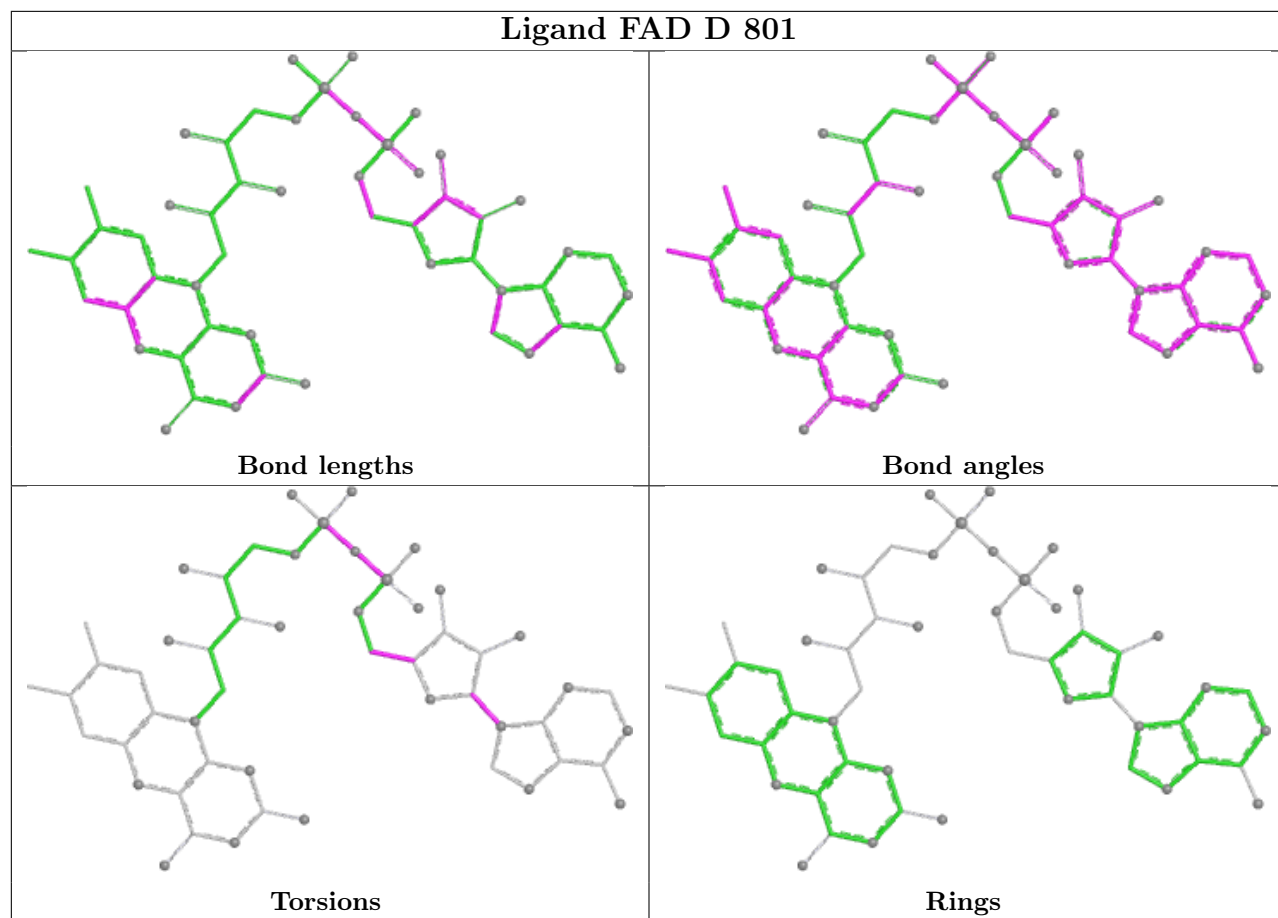
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

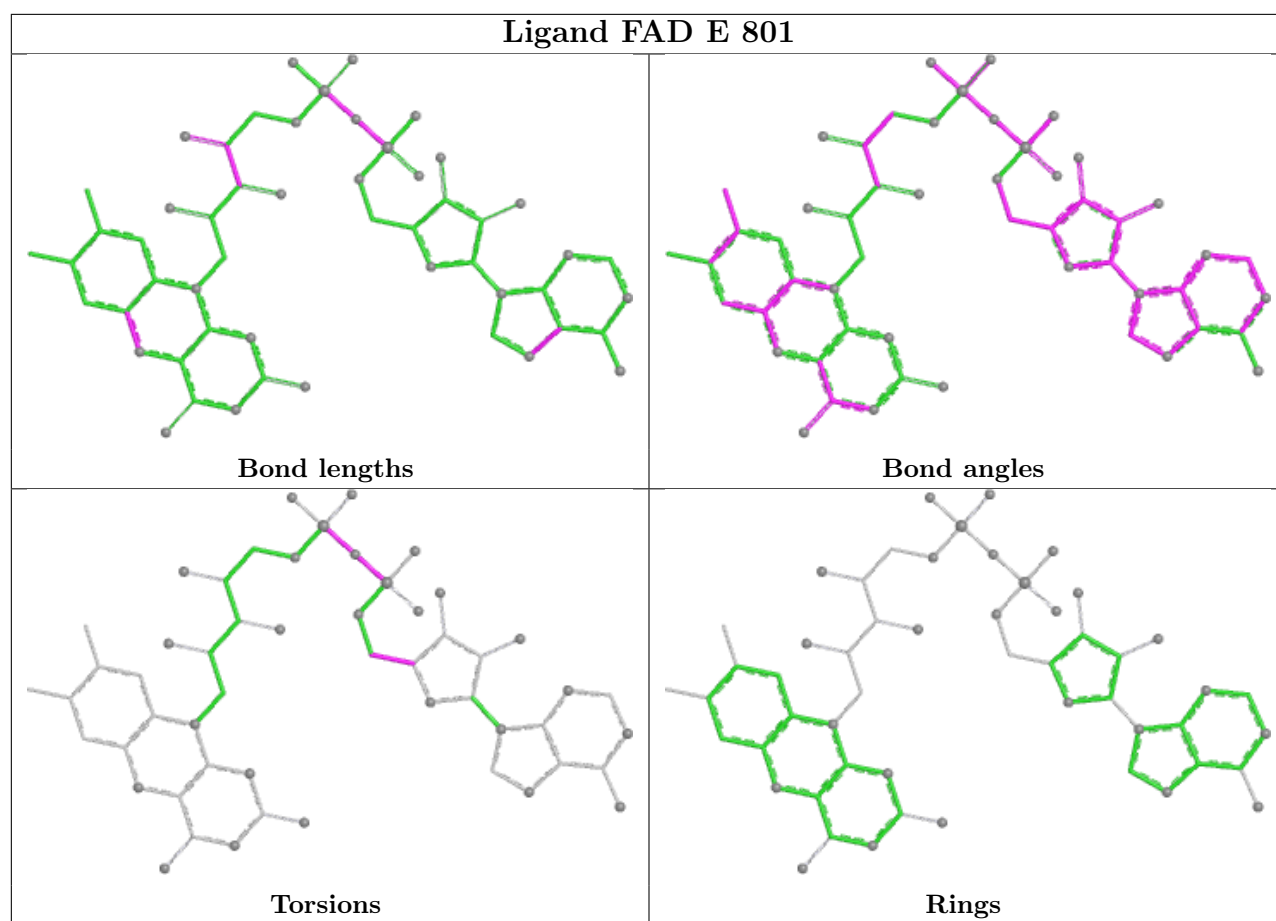




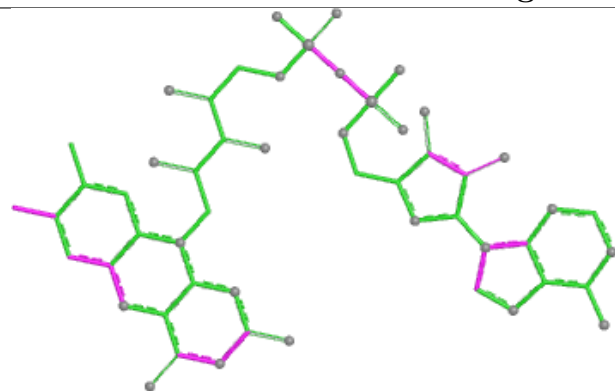




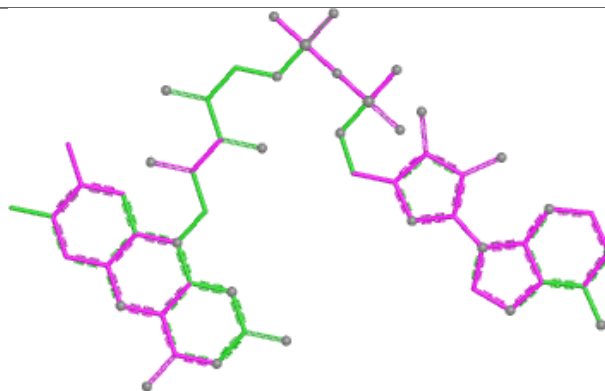




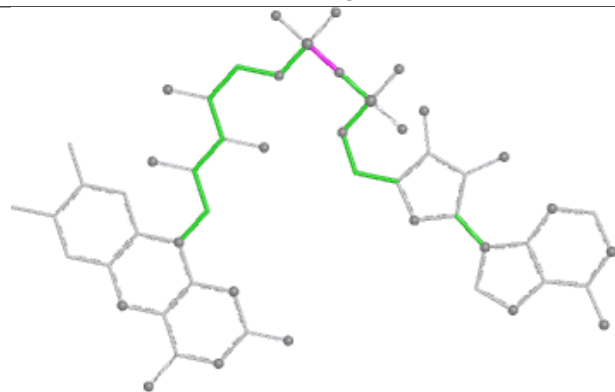
Ligand FAD B 801



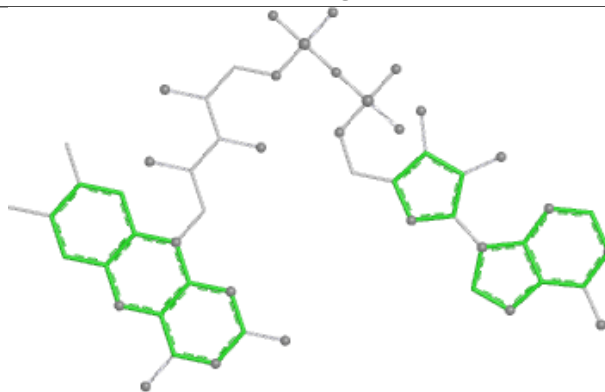
Bond lengths



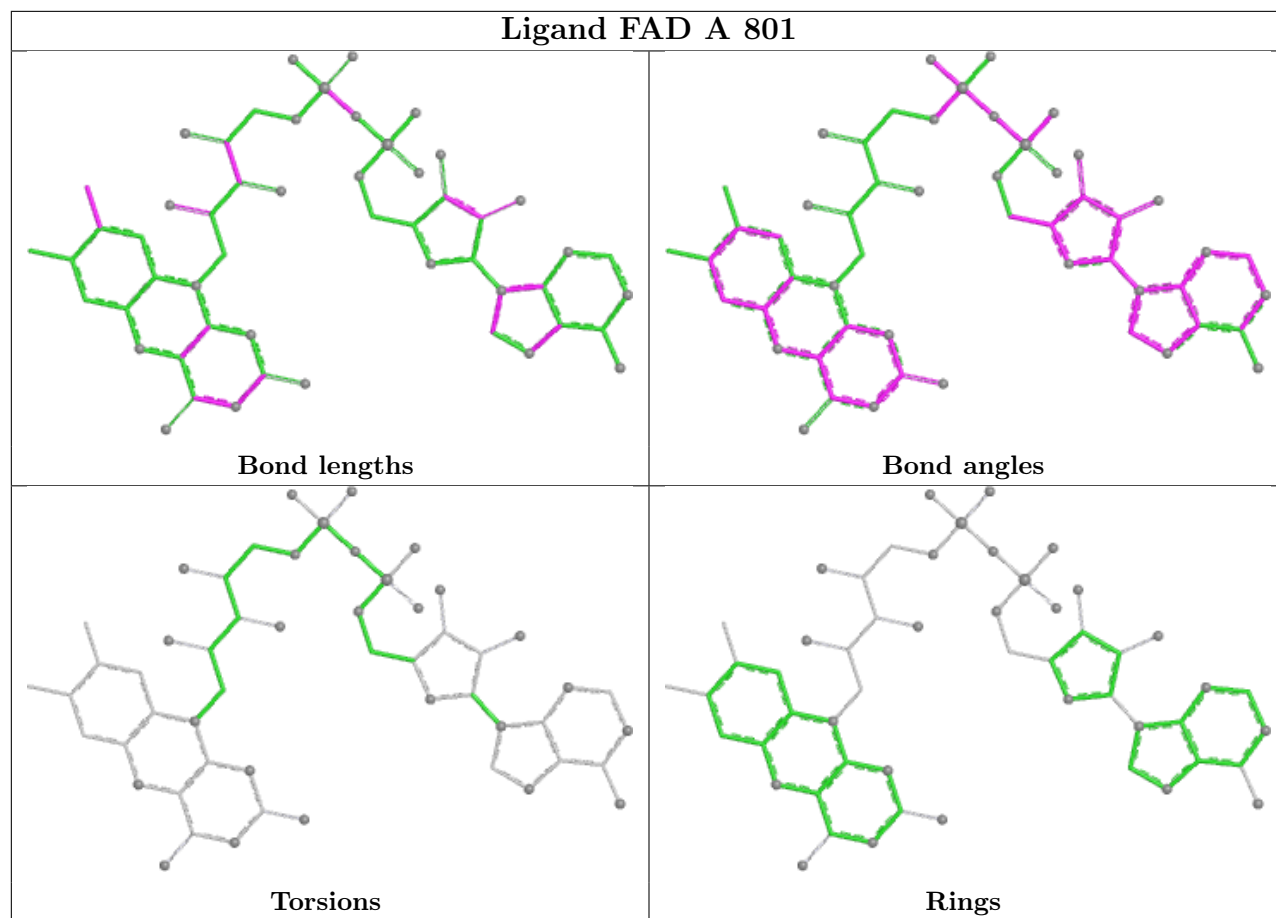
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	577/623 (92%)	0.33	35 (6%)	27	29	10, 32, 56, 75	1 (0%)
1	B	577/623 (92%)	0.28	24 (4%)	40	42	9, 33, 54, 77	2 (0%)
1	C	577/623 (92%)	0.59	33 (5%)	29	31	11, 38, 57, 83	2 (0%)
1	D	577/623 (92%)	0.44	33 (5%)	29	31	12, 36, 57, 77	2 (0%)
1	E	577/623 (92%)	0.58	38 (6%)	24	26	13, 39, 59, 81	2 (0%)
1	F	577/623 (92%)	0.65	33 (5%)	29	31	13, 40, 59, 83	1 (0%)
1	G	577/623 (92%)	0.45	27 (4%)	36	38	12, 36, 56, 78	3 (0%)
1	H	577/623 (92%)	0.34	31 (5%)	31	33	11, 35, 53, 78	3 (0%)
All	All	4616/4984 (92%)	0.46	254 (5%)	30	32	9, 36, 57, 83	16 (0%)

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	104	VAL	8.9
1	A	459	VAL	8.4
1	C	459	VAL	8.0
1	B	459	VAL	7.9
1	D	104	VAL	7.7
1	G	45	ILE	7.6
1	H	132	GLN	7.6
1	C	104	VAL	7.4
1	H	104	VAL	7.2
1	F	459	VAL	7.2
1	E	104	VAL	7.1
1	D	459	VAL	6.8
1	E	459	VAL	6.7
1	B	104	VAL	6.3
1	E	619	THR	6.2
1	G	299	HIS	6.2

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Mol	Chain	Res	Type	RSRZ
1	E	458	ALA	6.2
1	B	619	THR	6.2
1	C	132	GLN	6.1
1	C	619	THR	5.9
1	H	417	MET	5.9
1	A	104	VAL	5.8
1	D	458	ALA	5.7
1	F	44	ASP	5.7
1	F	619	THR	5.6
1	A	458	ALA	5.6
1	G	104	VAL	5.5
1	G	619	THR	5.5
1	E	132	GLN	5.5
1	D	132	GLN	5.4
1	D	619	THR	5.4
1	E	43	MET	5.2
1	G	132	GLN	5.2
1	H	619	THR	5.2
1	B	458	ALA	5.1
1	A	389	LEU	4.8
1	H	458	ALA	4.7
1	C	342	PRO	4.7
1	F	45	ILE	4.7
1	B	45	ILE	4.7
1	B	43	MET	4.6
1	C	44	ASP	4.6
1	B	132	GLN	4.6
1	H	459	VAL	4.6
1	C	45	ILE	4.6
1	G	44	ASP	4.6
1	G	459	VAL	4.5
1	H	43	MET	4.5
1	E	45	ILE	4.4
1	H	45	ILE	4.4
1	B	454	PHE	4.4
1	C	458	ALA	4.4
1	A	619	THR	4.4
1	E	385	THR	4.3
1	H	456	TYR	4.3
1	H	44	ASP	4.2
1	G	43	MET	4.2
1	B	456	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	460	GLN	4.2
1	F	460	GLN	4.2
1	D	454	PHE	4.2
1	A	45	ILE	4.1
1	F	43	MET	4.0
1	D	389	LEU	3.9
1	A	460	GLN	3.9
1	A	43	MET	3.9
1	G	454	PHE	3.9
1	C	456	TYR	3.9
1	C	389	LEU	3.8
1	C	618	PHE	3.8
1	D	43	MET	3.8
1	G	82	SER	3.7
1	F	618	PHE	3.7
1	G	618	PHE	3.7
1	A	390	THR	3.7
1	H	121	LEU	3.7
1	B	342	PRO	3.7
1	G	458	ALA	3.7
1	F	546	VAL	3.6
1	A	456	TYR	3.6
1	B	44	ASP	3.6
1	B	618	PHE	3.6
1	A	381	THR	3.6
1	F	458	ALA	3.6
1	B	460	GLN	3.6
1	D	44	ASP	3.5
1	E	454	PHE	3.5
1	F	342	PRO	3.5
1	H	342	PRO	3.5
1	F	547	LEU	3.4
1	G	456	TYR	3.4
1	E	44	ASP	3.4
1	C	547	LEU	3.3
1	C	454	PHE	3.3
1	E	618	PHE	3.3
1	E	460	GLN	3.3
1	D	45	ILE	3.3
1	C	43	MET	3.3
1	C	460	GLN	3.3
1	E	342	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	100	ILE	3.2
1	H	344	ASN	3.2
1	D	385	THR	3.2
1	H	454	PHE	3.2
1	C	343	ALA	3.1
1	H	81	ASP	3.1
1	H	618	PHE	3.1
1	D	547	LEU	3.1
1	E	389	LEU	3.1
1	D	456	TYR	3.1
1	A	401	THR	3.0
1	A	454	PHE	3.0
1	A	44	ASP	3.0
1	B	548	HIS	3.0
1	H	343	ALA	3.0
1	B	389	LEU	3.0
1	E	455	SER	3.0
1	D	344	ASN	3.0
1	F	456	TYR	3.0
1	D	388	GLU	3.0
1	F	457	GLY	3.0
1	E	456	TYR	3.0
1	G	455	SER	2.9
1	H	99	ASN	2.9
1	F	548	HIS	2.9
1	D	342	PRO	2.9
1	F	389	LEU	2.9
1	B	457	GLY	2.9
1	F	100	ILE	2.9
1	H	186	ASP	2.9
1	D	384	GLY	2.9
1	B	343	ALA	2.8
1	A	547	LEU	2.8
1	H	547	LEU	2.8
1	F	340	PRO	2.8
1	E	99	ASN	2.8
1	F	178	GLU	2.8
1	A	618	PHE	2.8
1	B	121	LEU	2.8
1	E	545	LEU	2.8
1	A	342	PRO	2.8
1	C	310	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	385	THR	2.7
1	F	454	PHE	2.7
1	D	546	VAL	2.7
1	G	343	ALA	2.7
1	E	547	LEU	2.7
1	E	457	GLY	2.7
1	F	268	THR	2.6
1	A	548	HIS	2.6
1	E	548	HIS	2.6
1	A	457	GLY	2.6
1	E	343	ALA	2.6
1	A	345	PRO	2.6
1	G	121	LEU	2.6
1	D	457	GLY	2.6
1	H	341	ASN	2.6
1	C	383	ARG	2.6
1	F	101	ASP	2.6
1	H	345	PRO	2.6
1	C	457	GLY	2.5
1	A	99	ASN	2.5
1	F	81	ASP	2.5
1	D	453	ALA	2.5
1	C	160	VAL	2.5
1	A	344	ASN	2.5
1	H	561	GLU	2.5
1	C	400	SER	2.5
1	D	345	PRO	2.5
1	B	81	ASP	2.4
1	F	421	GLU	2.4
1	H	460	GLN	2.4
1	H	542	GLU	2.4
1	D	121	LEU	2.4
1	B	178	GLU	2.4
1	H	269	ASP	2.4
1	F	343	ALA	2.4
1	G	457	GLY	2.4
1	A	81	ASP	2.4
1	E	386	PRO	2.4
1	G	342	PRO	2.4
1	A	387	GLY	2.4
1	E	232	GLY	2.4
1	B	546	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	345	PRO	2.4
1	D	618	PHE	2.3
1	H	347	GLU	2.3
1	G	338	GLY	2.3
1	G	389	LEU	2.3
1	C	81	ASP	2.3
1	B	82	SER	2.3
1	E	82	SER	2.3
1	C	548	HIS	2.3
1	E	390	THR	2.3
1	B	186	ASP	2.3
1	C	338	GLY	2.3
1	D	455	SER	2.3
1	C	345	PRO	2.3
1	C	390	THR	2.3
1	C	186	ASP	2.3
1	E	299	HIS	2.2
1	G	548	HIS	2.2
1	H	548	HIS	2.2
1	E	382	ILE	2.2
1	G	345	PRO	2.2
1	A	341	ASN	2.2
1	F	187	ASP	2.2
1	A	494	ALA	2.2
1	B	310	GLU	2.2
1	A	546	VAL	2.2
1	G	460	GLN	2.2
1	E	400	SER	2.2
1	D	99	ASN	2.2
1	F	385	THR	2.2
1	E	546	VAL	2.2
1	D	178	GLU	2.2
1	H	457	GLY	2.2
1	C	188	ALA	2.2
1	D	343	ALA	2.2
1	F	233	GLN	2.2
1	A	383	ARG	2.2
1	C	421	GLU	2.1
1	E	561	GLU	2.1
1	F	232	GLY	2.1
1	F	338	GLY	2.1
1	D	545	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	82	SER	2.1
1	C	312	LYS	2.1
1	A	452	ASP	2.1
1	A	561	GLU	2.1
1	E	81	ASP	2.1
1	E	346	PRO	2.1
1	D	548	HIS	2.1
1	D	383	ARG	2.1
1	C	392	SER	2.1
1	A	386	PRO	2.1
1	G	160	VAL	2.1
1	H	389	LEU	2.1
1	A	461	GLN	2.1
1	F	390	THR	2.1
1	F	617	PRO	2.1
1	H	340	PRO	2.1
1	E	387	GLY	2.1
1	E	312	LYS	2.1
1	C	546	VAL	2.1
1	G	546	VAL	2.1
1	A	400	SER	2.1
1	E	358	GLU	2.0
1	F	121	LEU	2.0
1	D	386	PRO	2.0
1	D	390	THR	2.0
1	A	388	GLU	2.0
1	G	310	GLU	2.0
1	E	543	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 oligosaccharides in this entry.

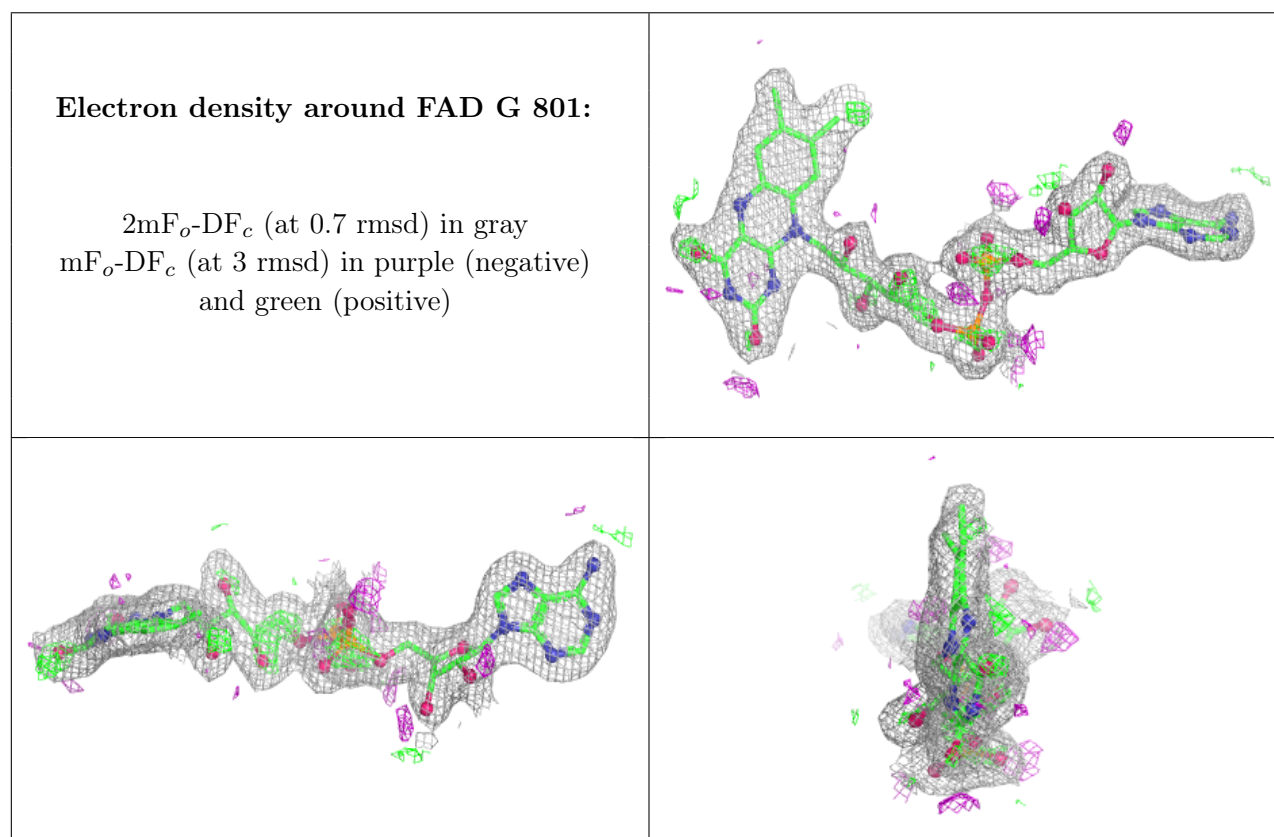
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

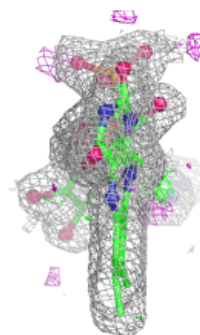
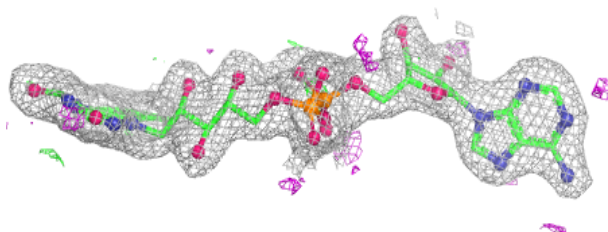
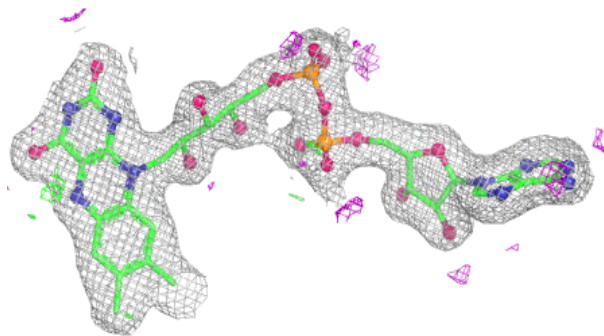
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	G	801	53/53	0.94	0.09	20,24,30,33	0
2	FAD	F	801	53/53	0.95	0.08	16,28,33,35	0
2	FAD	C	801	53/53	0.95	0.07	23,29,35,43	0
2	FAD	E	801	53/53	0.96	0.07	21,30,35,38	0
2	FAD	H	801	53/53	0.96	0.08	19,27,31,32	0
2	FAD	A	801	53/53	0.97	0.06	20,24,30,35	0
2	FAD	D	801	53/53	0.97	0.07	23,27,31,35	0
2	FAD	B	801	53/53	0.97	0.06	18,23,28,34	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.

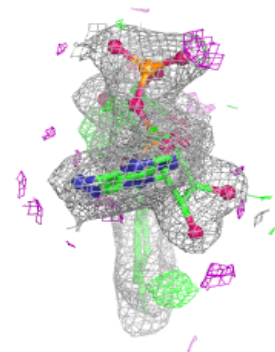
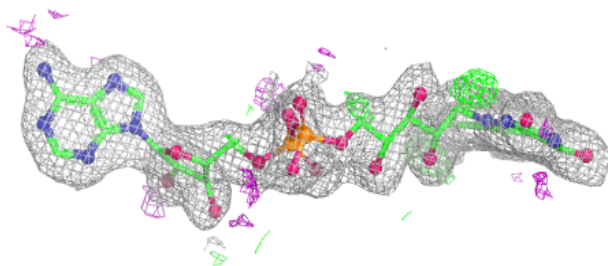
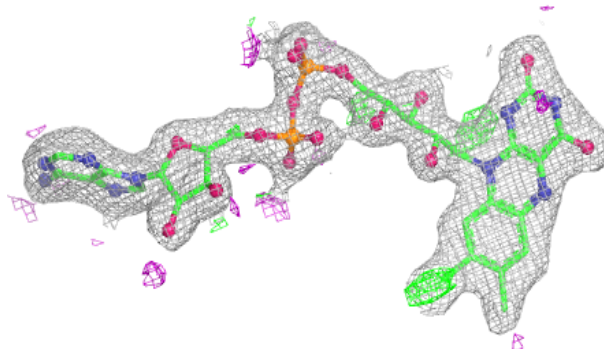


Electron density around FAD F 801:

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

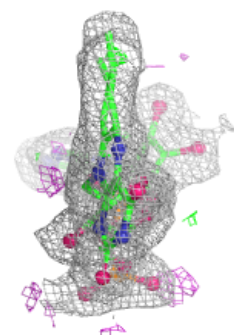
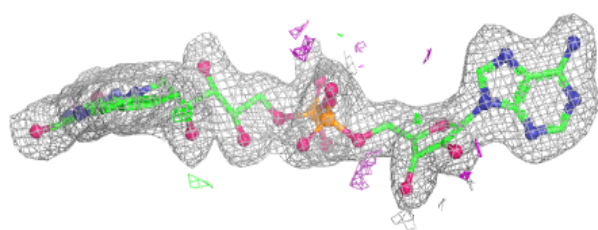
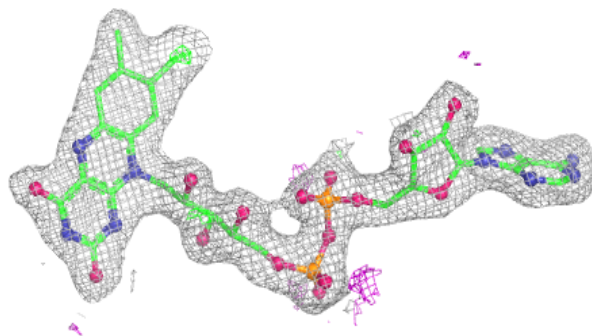
**Electron density around FAD C 801:**

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

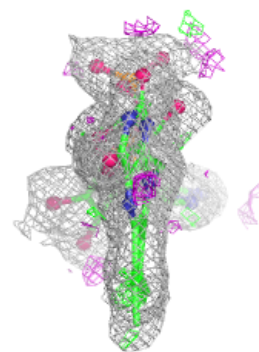
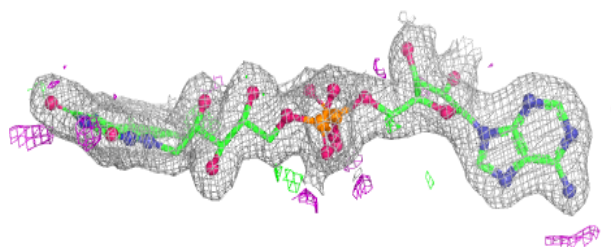
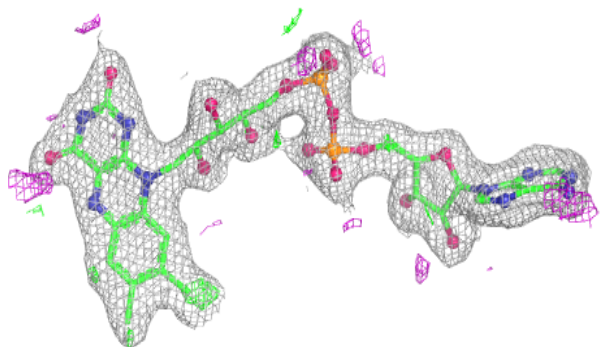


Electron density around FAD E 801:

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

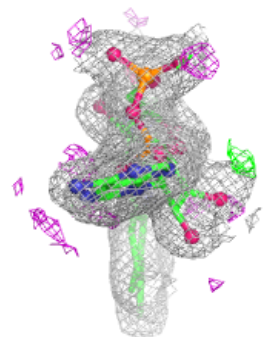
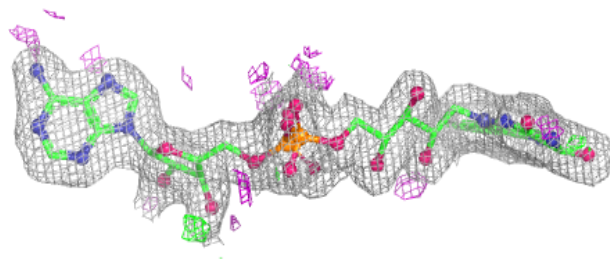
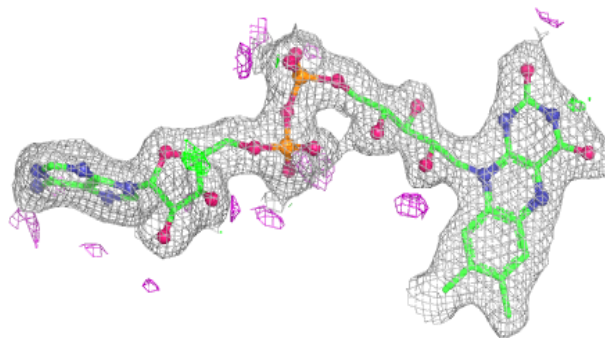
**Electron density around FAD H 801:**

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

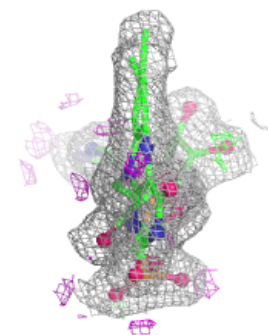
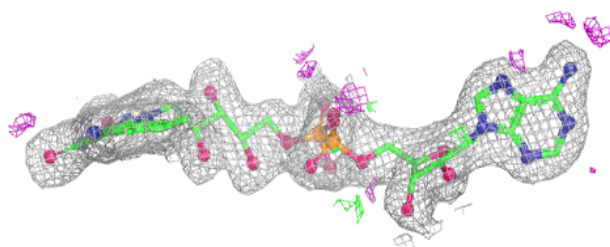
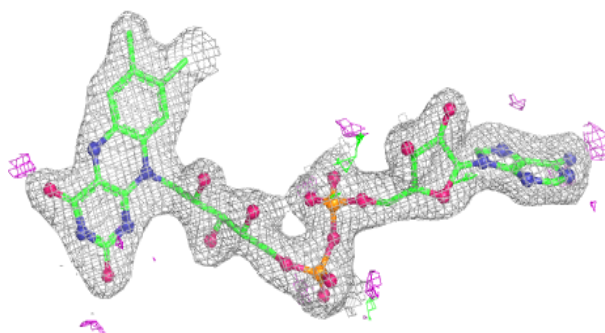


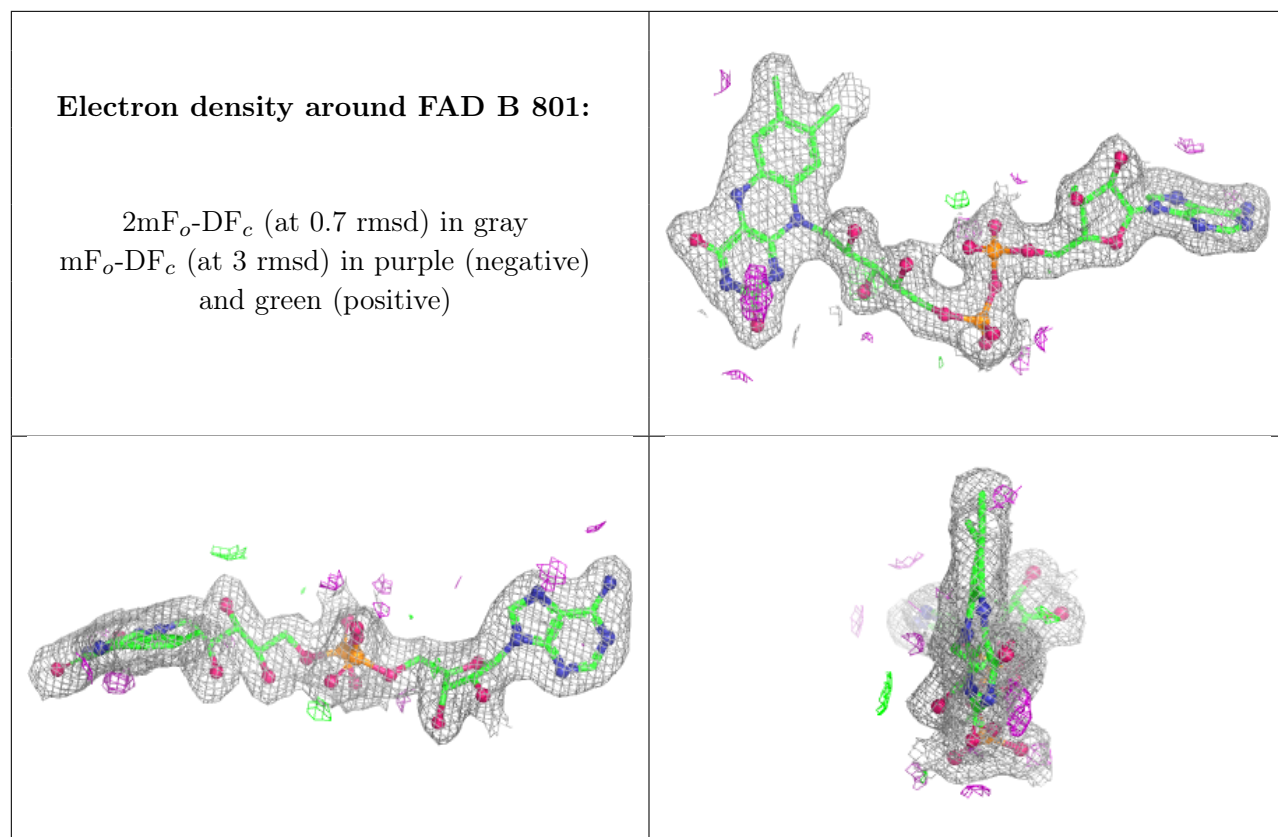
Electron density around FAD A 801:

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

**Electron density around FAD D 801:**

$2mF_o-DF_c$ (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.