Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 11:49 PM EDT

PDB ID	:	3BG7
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:

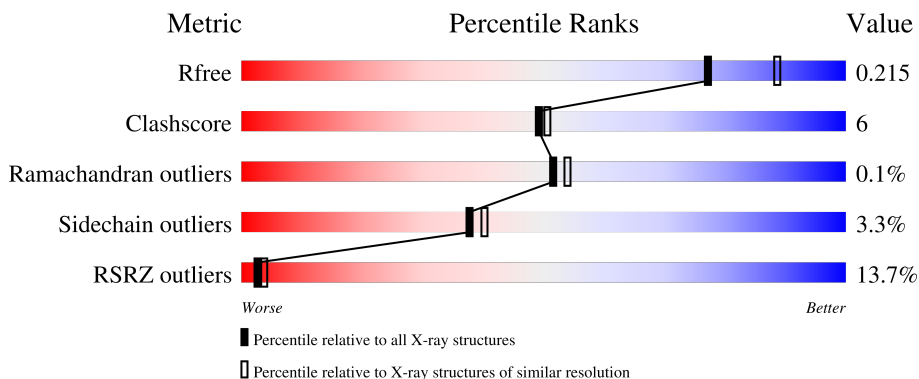|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 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.
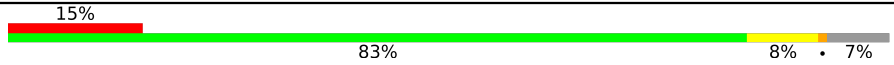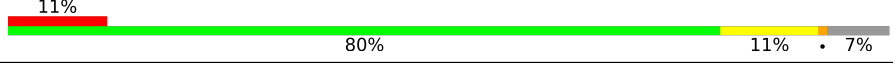
Metric	Percentile Ranks	Value
Rfree		0.215
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		3.3%
RSRZ outliers		13.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	11% / 81% / 11% · 7%
1	B	623	10% / 80% / 11% · 7%
1	C	623	13% / 81% / 10% · 7%
1	D	623	12% / 82% / 9% · 7%
1	E	623	16% / 83% / 9% · 7%

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Mol	Chain	Length	Quality of chain
1	F	623	15% ■■■■ 83% 8% · 7%
1	G	623	13% ■■■ 83% 8% · 7%
1	H	623	11% ■■ 80% 11% · 7%

2 Entity 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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

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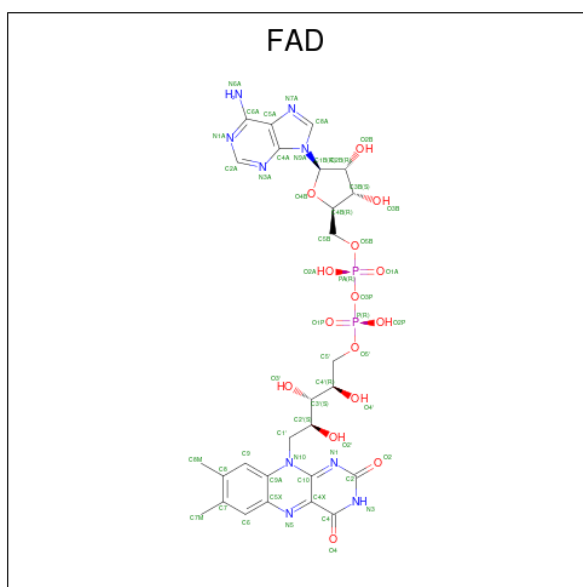
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G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

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
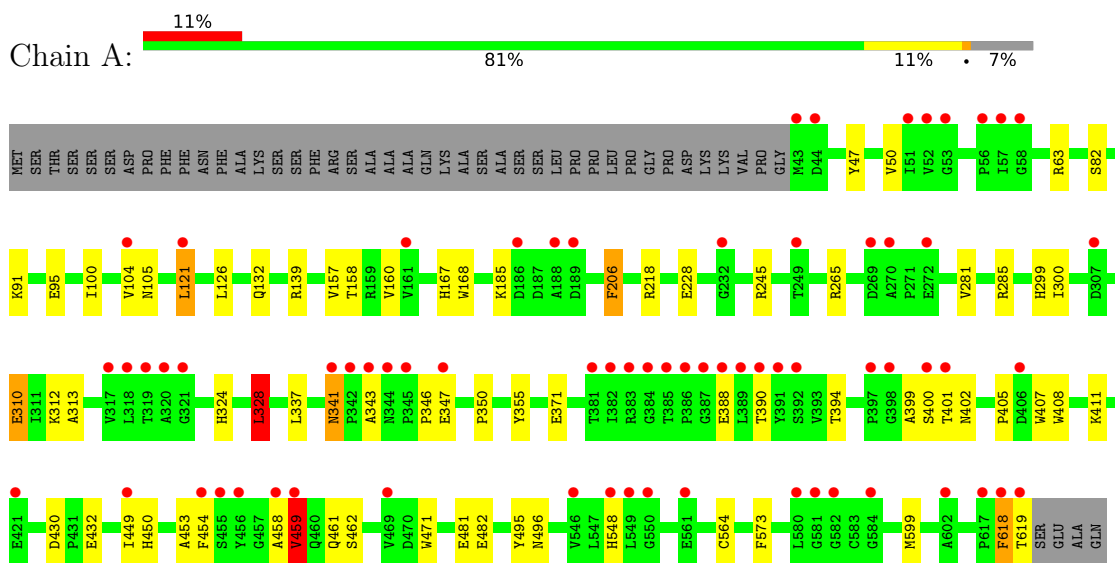
Chain A:

• Molecule 1: Pyranose oxidase

Chain B:

• Molecule 1: Pyranose oxidase

Chain C:

• Molecule 1: Pyranose oxidase
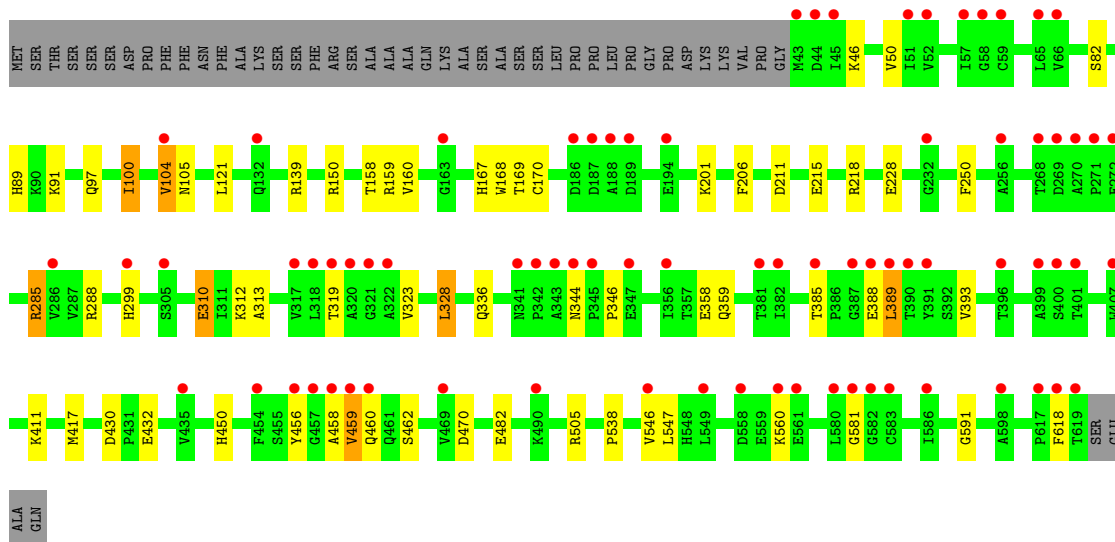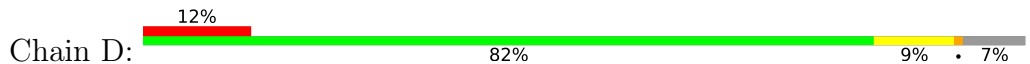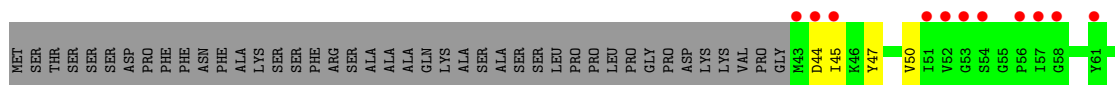
Chain D:
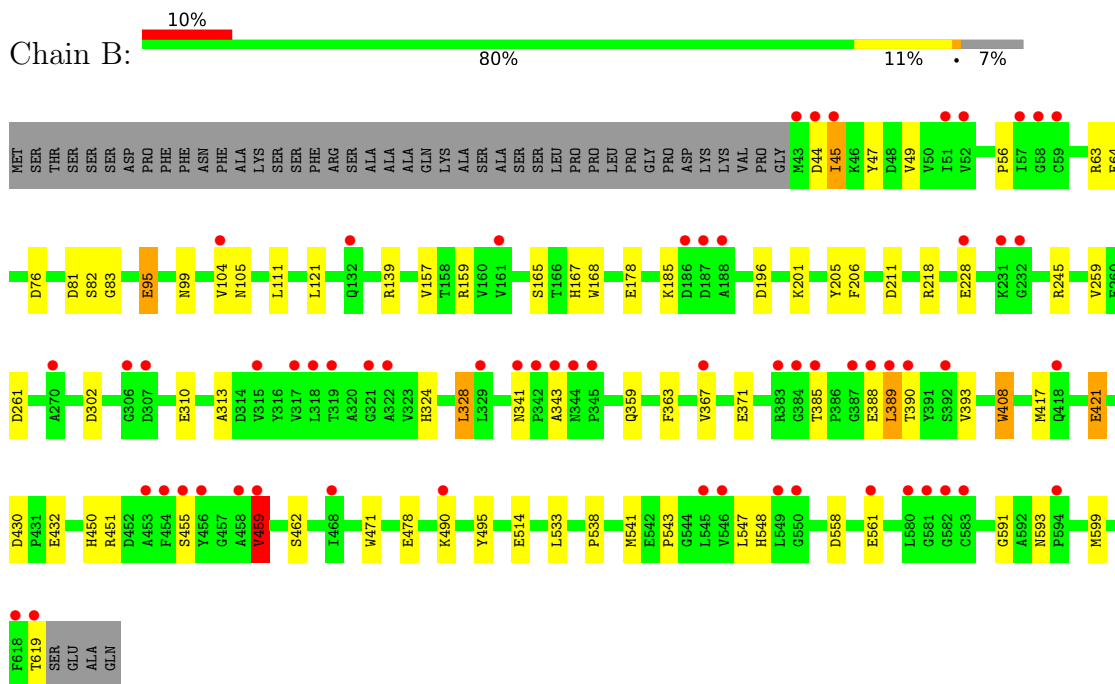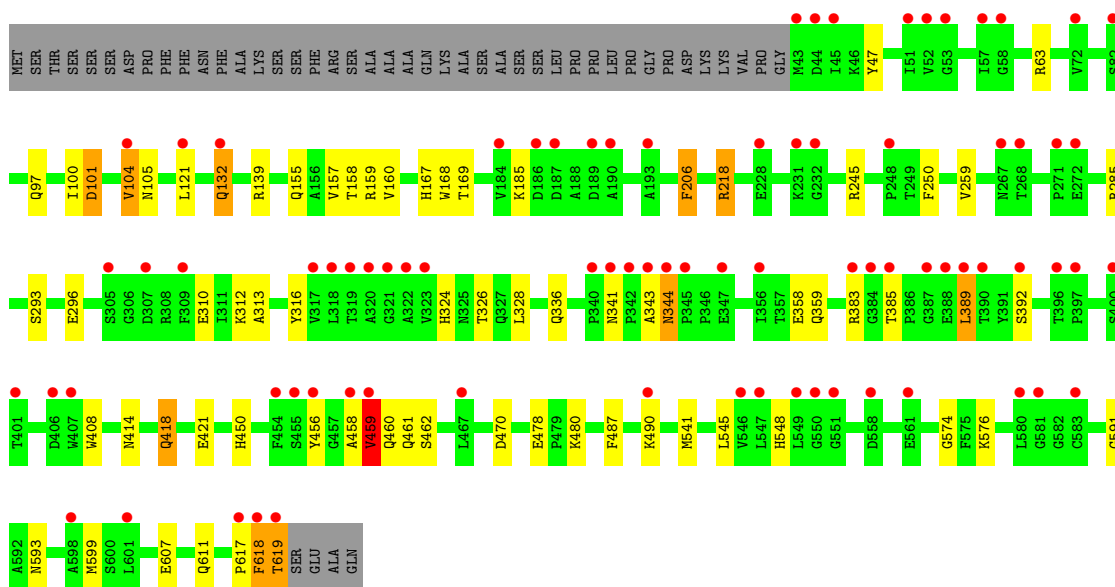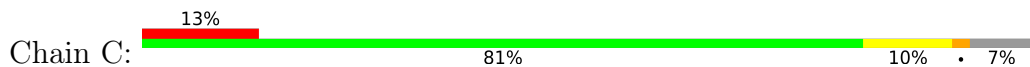
• Molecule 1: Pyranose oxidase

Chain E:

• Molecule 1: Pyranose oxidase

Chain F:

• Molecule 1: Pyranose oxidase

Chain G:

• Molecule 1: Pyranose oxidase

Chain H:
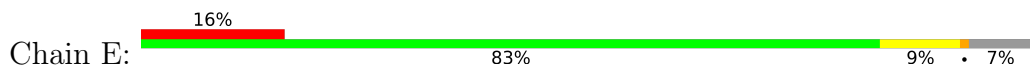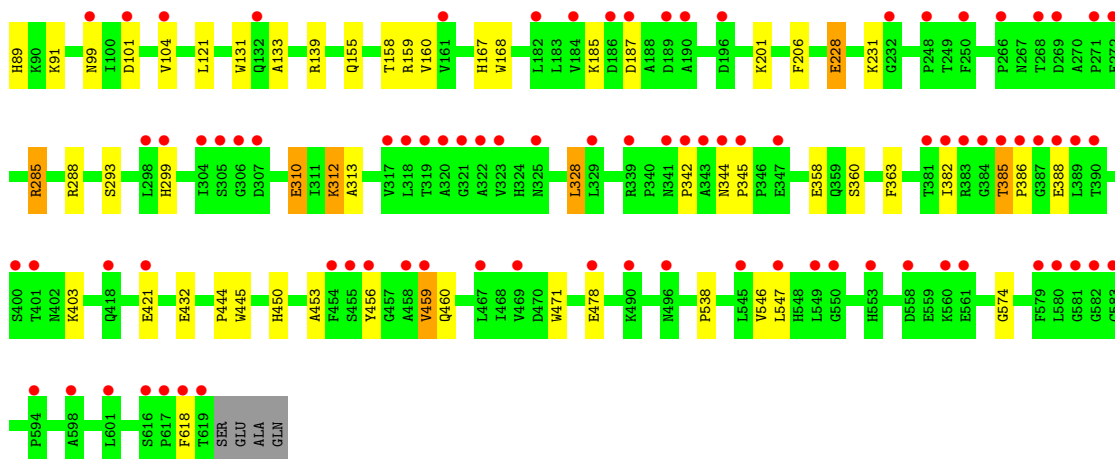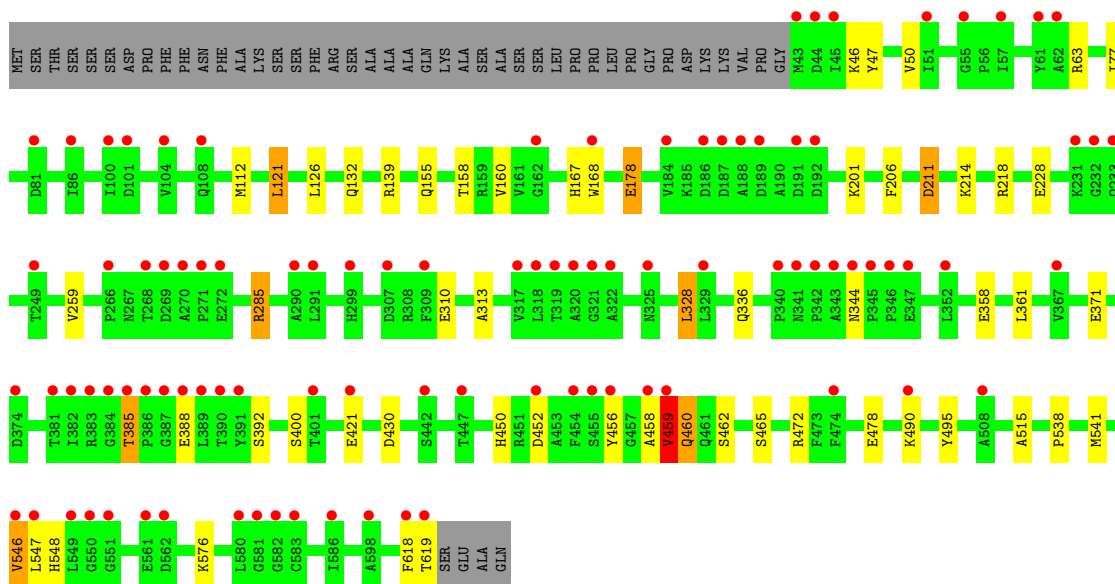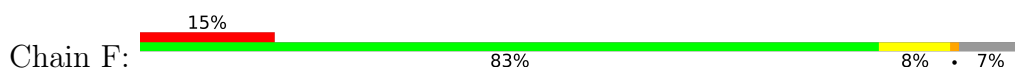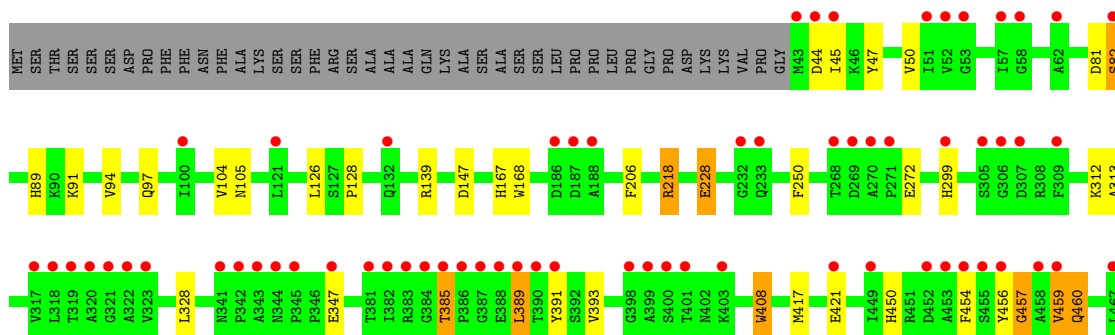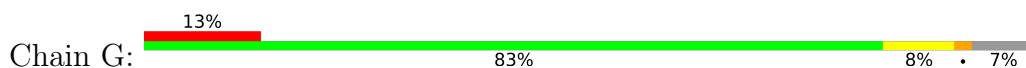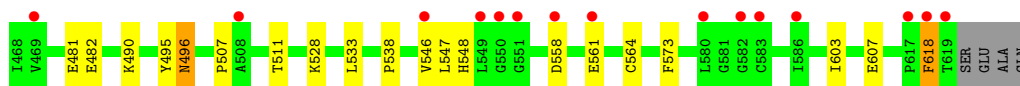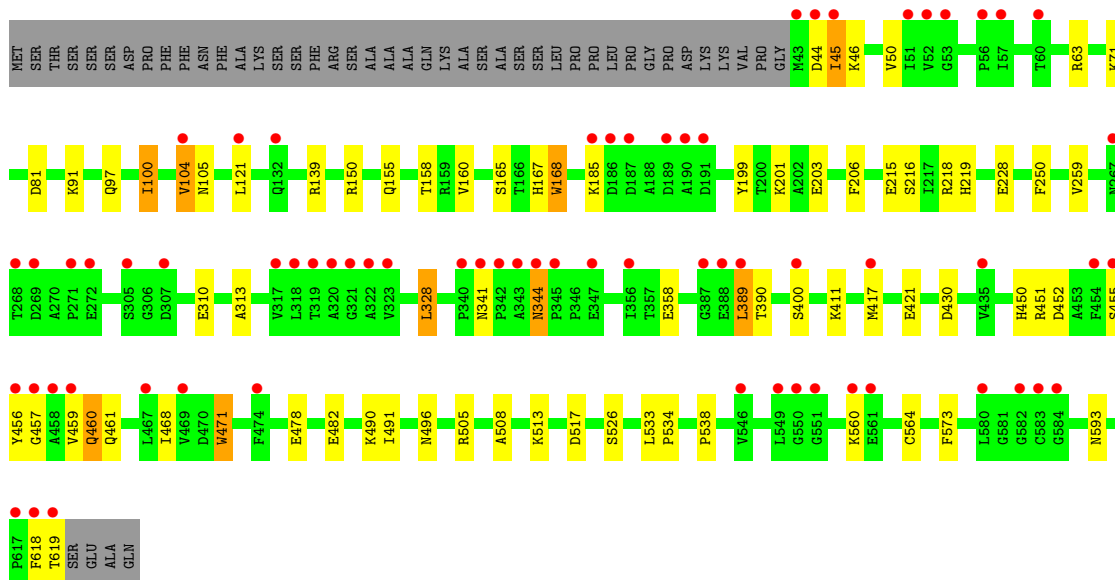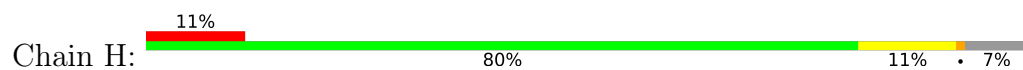
4 Data and refinement statistics ⓘ

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) 99.1 (29.72-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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 (1.02%)	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 , 56.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	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.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.12	11/4661 (0.2%)	0.97	11/6337 (0.2%)
1	B	1.13	10/4661 (0.2%)	1.00	17/6337 (0.3%)
1	C	0.99	5/4661 (0.1%)	0.90	9/6337 (0.1%)
1	D	1.01	6/4661 (0.1%)	0.90	8/6337 (0.1%)
1	E	0.98	9/4661 (0.2%)	0.86	6/6337 (0.1%)
1	F	0.95	7/4661 (0.2%)	0.87	5/6337 (0.1%)
1	G	1.06	9/4661 (0.2%)	0.91	7/6337 (0.1%)
1	H	1.04	9/4661 (0.2%)	0.92	6/6337 (0.1%)
All	All	1.04	66/37288 (0.2%)	0.92	69/50696 (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 (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	GLU	CG-CD	10.91	1.68	1.51
1	D	310	GLU	CG-CD	10.02	1.67	1.51
1	D	310	GLU	CB-CG	8.87	1.69	1.52
1	A	310	GLU	CB-CG	8.15	1.67	1.52
1	E	310	GLU	CG-CD	8.00	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	228	GLU	CG-CD	7.88	1.63	1.51
1	A	310	GLU	CG-CD	7.59	1.63	1.51
1	G	482	GLU	CG-CD	7.38	1.63	1.51
1	B	421	GLU	CB-CG	6.87	1.65	1.52
1	F	228	GLU	CG-CD	6.87	1.62	1.51
1	H	310	GLU	CG-CD	6.85	1.62	1.51
1	A	432	GLU	CD-OE2	6.84	1.33	1.25
1	E	310	GLU	CB-CG	6.78	1.65	1.52
1	D	482	GLU	CG-CD	6.58	1.61	1.51
1	F	310	GLU	CG-CD	6.51	1.61	1.51
1	G	421	GLU	CB-CG	6.49	1.64	1.52
1	F	310	GLU	CB-CG	6.47	1.64	1.52
1	D	228	GLU	CG-CD	6.45	1.61	1.51
1	G	228	GLU	CG-CD	6.39	1.61	1.51
1	H	482	GLU	CG-CD	6.32	1.61	1.51
1	E	312	LYS	CD-CE	6.30	1.67	1.51
1	E	228	GLU	CG-CD	6.23	1.61	1.51
1	B	310	GLU	CB-CG	6.22	1.64	1.52
1	A	482	GLU	CG-CD	6.21	1.61	1.51
1	H	228	GLU	CB-CG	6.18	1.63	1.52
1	B	310	GLU	CG-CD	6.16	1.61	1.51
1	G	460	GLN	CB-CG	6.16	1.69	1.52
1	A	371	GLU	CD-OE1	6.11	1.32	1.25
1	A	228	GLU	CG-CD	6.04	1.61	1.51
1	G	82	SER	CB-OG	6.03	1.50	1.42
1	A	228	GLU	CD-OE1	6.01	1.32	1.25
1	C	310	GLU	CB-CG	5.98	1.63	1.52
1	E	421	GLU	CG-CD	5.97	1.60	1.51
1	A	371	GLU	CG-CD	5.74	1.60	1.51
1	B	514	GLU	CG-CD	5.70	1.60	1.51
1	D	432	GLU	CG-CD	5.62	1.60	1.51
1	C	421	GLU	CB-CG	5.62	1.62	1.52
1	G	347	GLU	CG-CD	5.59	1.60	1.51
1	F	371	GLU	CG-CD	5.58	1.60	1.51
1	A	139	ARG	CD-NE	-5.57	1.36	1.46
1	B	49	VAL	CB-CG2	5.56	1.64	1.52
1	C	310	GLU	CG-CD	5.52	1.60	1.51
1	A	355	TYR	CD2-CE2	-5.50	1.31	1.39
1	D	323	VAL	CB-CG2	5.48	1.64	1.52
1	C	101	ASP	CB-CG	5.41	1.63	1.51
1	H	508	ALA	CA-CB	5.41	1.63	1.52
1	E	421	GLU	CB-CG	5.40	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	310	GLU	CB-CG	5.39	1.62	1.52
1	B	371	GLU	CG-CD	5.33	1.59	1.51
1	G	94	VAL	CB-CG2	5.32	1.64	1.52
1	H	104	VAL	CB-CG2	-5.26	1.41	1.52
1	F	478	GLU	CG-CD	5.25	1.59	1.51
1	E	101	ASP	CB-CG	5.24	1.62	1.51
1	G	490	LYS	CD-CE	5.23	1.64	1.51
1	H	471	TRP	CB-CG	-5.22	1.40	1.50
1	E	432	GLU	CG-CD	5.21	1.59	1.51
1	B	478	GLU	CG-CD	5.21	1.59	1.51
1	H	478	GLU	CD-OE1	5.18	1.31	1.25
1	B	104	VAL	CB-CG2	-5.14	1.42	1.52
1	B	432	GLU	CD-OE2	5.12	1.31	1.25
1	G	421	GLU	CG-CD	5.09	1.59	1.51
1	F	178	GLU	CG-CD	5.08	1.59	1.51
1	C	132	GLN	CG-CD	5.03	1.62	1.51
1	F	478	GLU	CD-OE1	5.03	1.31	1.25
1	E	478	GLU	CD-OE1	5.03	1.31	1.25
1	A	347	GLU	CB-CG	5.02	1.61	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH2	-17.72	111.44	120.30
1	F	139	ARG	NE-CZ-NH2	-17.23	111.69	120.30
1	B	139	ARG	NE-CZ-NH2	-14.69	112.96	120.30
1	E	139	ARG	NE-CZ-NH2	-13.21	113.70	120.30
1	C	139	ARG	NE-CZ-NH2	-13.05	113.77	120.30
1	D	139	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	B	139	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	C	139	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	F	139	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	G	139	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	H	139	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	139	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	D	139	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	196	ASP	CB-CG-OD1	7.51	125.06	118.30
1	H	104	VAL	CB-CA-C	-7.38	97.38	111.40
1	B	261	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	139	ARG	CG-CD-NE	-7.18	96.71	111.80
1	B	245	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	H	139	ARG	NE-CZ-NH1	7.05	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($°$)	Ideal($°$)
1	E	139	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	B	211	ASP	CB-CG-OD1	6.91	124.52	118.30
1	G	139	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	218	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	104	VAL	CB-CA-C	-6.63	98.80	111.40
1	C	245	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	245	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	139	ARG	CD-NE-CZ	6.50	132.70	123.60
1	H	328	LEU	CA-CB-CG	6.41	130.04	115.30
1	D	288	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	470	ASP	CB-CG-OD1	6.15	123.84	118.30
1	H	81	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	C	218	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	302	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	599	MET	CG-SD-CE	5.98	109.77	100.20
1	B	328	LEU	CB-CG-CD1	5.96	121.13	111.00
1	G	147	ASP	CB-CG-OD1	5.90	123.61	118.30
1	H	417	MET	CG-SD-CE	-5.86	90.83	100.20
1	G	218	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	D	310	GLU	OE1-CD-OE2	-5.82	116.31	123.30
1	F	211	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	63	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	245	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	139	ARG	CB-CA-C	-5.70	99.00	110.40
1	C	101	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	451	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	470	ASP	CB-CG-OD1	5.60	123.34	118.30
1	E	288	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	139	ARG	CG-CD-NE	-5.54	100.17	111.80
1	B	111	LEU	CB-CG-CD1	-5.42	101.80	111.00
1	C	139	ARG	CB-CA-C	-5.40	99.59	110.40
1	E	310	GLU	OE1-CD-OE2	-5.40	116.83	123.30
1	G	139	ARG	CB-CA-C	-5.38	99.63	110.40
1	C	470	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	G	82	SER	CA-CB-OG	5.33	125.60	111.20
1	A	265	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	76	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	211	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	211	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	F	139	ARG	CG-CD-NE	-5.23	100.81	111.80
1	B	139	ARG	CD-NE-CZ	5.23	130.92	123.60
1	E	139	ARG	CB-CA-C	-5.18	100.04	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	337	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	A	63	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	139	ARG	CG-CD-NE	-5.08	101.14	111.80
1	B	82	SER	CB-CA-C	-5.08	100.46	110.10
1	F	139	ARG	CD-NE-CZ	5.08	130.71	123.60
1	A	328	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	265	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	G	139	ARG	CG-CD-NE	-5.02	101.26	111.80

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	58	0
1	B	4545	0	4387	77	0
1	C	4545	0	4387	67	0
1	D	4545	0	4387	52	0
1	E	4545	0	4387	60	0
1	F	4545	0	4387	52	0
1	G	4545	0	4387	54	0
1	H	4545	0	4387	62	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
3	C	209	0	0	3	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	5	0
3	H	256	0	0	2	0
All	All	38641	0	35322	416	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 (416) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1.19	1.05
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:63:ARG:HD2	1:F:259:VAL:O	1.85	0.76
1:B:393:VAL:N	1:B:417:MET:HE2	1.99	0.76
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.69	0.75
1:B:389:LEU:HD13	1:B:389:LEU:H	1.53	0.74
1:E:459:VAL:CG1	1:F:121:LEU:HB3	2.18	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: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:G:393:VAL:H	1:G:417:MET:CE	2.07	0.67
1:C:101:ASP:O	1:C:104:VAL:HG23	1.95	0.67
1:E:459:VAL:HG12	1:F:121:LEU:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:G:393:VAL:H	1:G:417:MET:HE2	1.63	0.64
1:C:459:VAL:HG13	1:D:121:LEU:CB	2.27	0.63
1:B:541:MET:HE3	3:B:959:HOH:O	1.97	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: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:H:201:LYS:NZ	3:H:906:HOH:O	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:E:91:LYS:NZ	3:E:822:HOH:O	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:564:CYS:HG	1:H:573:PHE:HE2	1.55	0.54
1:C:343:ALA:C	1:C:344:ASN:HD22	2.11	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: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:A:564:CYS:HG	1:A:573:PHE:HE2	1.56	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: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:D:393:VAL:H	1:D:417:MET:CE	2.22	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.92	0.50
1:B:167:HIS:CE1	2:B:801:FAD:C8M	2.88	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:H:45:ILE:C	1:H:45:ILE:HD12	2.32	0.50
1:A:299:HIS:HD1	1:A:310:GLU:CD	2.14	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:D:336:GLN:HB2	1:D:346:PRO:HG3	1.95	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: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:D:218:ARG:HG3	1:D:430:ASP:OD2	2.12	0.48
1:B:81:ASP:OD1	1:B:81:ASP:C	2.51	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: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: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:F:201:LYS:NZ	3:F:964:HOH:O	2.46	0.47
1:C:312:LYS:HD2	1:C:316:TYR:OH	2.13	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:E:344:ASN:N	1:E:345:PRO:CD	2.77	0.47
1:G:44:ASP:OD1	1:G:45:ILE:HG13	2.14	0.47
1:G:393:VAL:H	1:G:417:MET:HE1	1.78	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:G:459:VAL:O	1:G:460:GLN:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:201:LYS:NZ	3:D:881:HOH:O	2.28	0.46
1:E:293:SER:HA	1:E:574:GLY:O	2.15	0.46
1:F:126:LEU:HD13	1:F:132:GLN:CG	2.45	0.46
1:B:459:VAL:O	1:B:462:SER:HB3	2.16	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:G:457:GLY:C	1:G:459:VAL:H	2.19	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: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
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: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:G:104:VAL:HG21	1:G:454:PHE:C	2.36	0.45
1:G:167:HIS:C	1:G:167:HIS:CD2	2.89	0.45
1:H:456:TYR:HD1	1:H:460:GLN:HB3	1.79	0.45
1:A:104:VAL:HG22	1:A:453:ALA:C	2.37	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:G:618:PHE:C	1:G:618:PHE:CD1	2.90	0.45
1:B:159:ARG:HA	2:B:801:FAD:O2B	2.17	0.45
1:E:131:TRP:CH2	1:E:133:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:CD1	1:A:132:GLN:CG	2.95	0.44
1:B:167:HIS:CD2	1:B:167:HIS:C	2.90	0.44
1:E:342:PRO:C	1:E:344:ASN:H	2.20	0.44
1:H:97:GLN:HG3	1:H:250:PHE:CD2	2.52	0.44
1:A:206:PHE:CE2	1:A:599:MET:HE3	2.53	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:A:158:THR:HG22	1:A:160:VAL:HG22	2.00	0.44
1:A:341:ASN:HD22	1:A:341:ASN:C	2.21	0.44
1:D:358:GLU:OE1	1:D:546:VAL:HG13	2.17	0.44
1:H:344:ASN:CG	1:H:344:ASN:O	2.55	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:B:121:LEU:HD21	1:C:121:LEU:HD23	1.99	0.44
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.83	0.44
1:C:408:TRP:CD1	1:C:408:TRP:C	2.90	0.44
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.83	0.43
1:G:564:CYS:HG	1:G:573:PHE:HE2	1.66	0.43
1:C:344:ASN:N	1:C:344:ASN:ND2	2.64	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:A:95:GLU:OE1	1:B:495:TYR:OH	2.29	0.43
1:B:547:LEU:CD1	2:B:801:FAD:HM83	2.48	0.43
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:328:LEU:HD12	1:F:328:LEU:C	2.37	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:408:TRP:CD1	1:B:408:TRP:C	2.92	0.43
1:C:618:PHE:CD1	1:C:618:PHE:C	2.92	0.43
1:B:363:PHE:HA	1:B:471:TRP:O	2.19	0.43
1:C:541:MET:HE2	1:C:545:LEU:HD23	2.01	0.43
1:F:158:THR:HG22	1:F:160:VAL:HG22	2.01	0.43
1:H:100:ILE:HD13	1:H:100:ILE:C	2.39	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:A:341:ASN:HD22	1:A:343:ALA:N	2.07	0.43
1:E:201:LYS:NZ	3:E:945:HOH:O	2.47	0.43
1:E:363:PHE:HA	1:E:471:TRP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:HIS:NE2	2:E:801:FAD:HM81	2.10	0.42
1:F:285:ARG:HA	1:F:328:LEU:HD13	1.99	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:D:359:GLN:NE2	1:D:591:GLY:C	2.73	0.42
1:E:382:ILE:N	1:E:382:ILE:HD12	2.34	0.42
1:H:165:SER:HA	1:H:168:TRP:CD1	2.54	0.42
1:H:459:VAL:HG12	1:H:460:GLN:N	2.34	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:359:GLN:HE21	1:C:591:GLY:C	2.23	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:G:408:TRP:CD1	1:G:408:TRP:C	2.93	0.41
1:H:199:TYR:O	1:H:203:GLU:HG3	2.20	0.41
1:A:459:VAL:HG22	1:B:121:LEU:HD13	2.03	0.41
1:A:459:VAL:HA	1:A:462:SER:HB2	2.02	0.41
1:A:618:PHE:C	1:A:618:PHE:CD1	2.93	0.41
1:C:155:GLN:NE2	1:C:358:GLU:OE2	2.49	0.41
1:D:215:GLU:O	1:D:411:LYS:NZ	2.54	0.41
1:D:547:LEU:HD12	2:D:801:FAD:HM83	2.01	0.41
1:C:618:PHE:C	1:C:618:PHE:HD1	2.24	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:H:44:ASP:HB3	1:H:46:LYS:H	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:343:ALA:C	1:C:344:ASN:ND2	2.73	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:H:45:ILE:C	1:H:45:ILE:CD1	2.89	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:H:452:ASP:C	1:H:452:ASP:OD1	2.59	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: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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	47	49
1	F	575/623 (92%)	560 (97%)	15 (3%)	0	100	100
1	G	575/623 (92%)	552 (96%)	22 (4%)	1 (0%)	47	49
1	H	575/623 (92%)	555 (96%)	19 (3%)	1 (0%)	47	49
All	All	4600/4984 (92%)	4442 (97%)	155 (3%)	3 (0%)	51	54

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	504/541 (93%)	487 (97%)	17 (3%)	37	39
1	B	504/541 (93%)	487 (97%)	17 (3%)	37	39
1	C	504/541 (93%)	487 (97%)	17 (3%)	37	39
1	D	504/541 (93%)	488 (97%)	16 (3%)	39	41
1	E	504/541 (93%)	488 (97%)	16 (3%)	39	41
1	F	504/541 (93%)	483 (96%)	21 (4%)	30	30
1	G	504/541 (93%)	491 (97%)	13 (3%)	46	50
1	H	504/541 (93%)	487 (97%)	17 (3%)	37	39
All	All	4032/4328 (93%)	3898 (97%)	134 (3%)	38	40

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	121	LEU
1	A	168	TRP
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	450	HIS
1	A	459	VAL
1	A	461	GLN
1	A	618	PHE
1	A	619	THR
1	B	44	ASP
1	B	45	ILE
1	B	95	GLU
1	B	168	TRP
1	B	185	LYS
1	B	206	PHE
1	B	328	LEU
1	B	385	THR
1	B	389	LEU
1	B	408	TRP
1	B	421	GLU
1	B	450	HIS
1	B	455	SER
1	B	459	VAL
1	B	490	LYS
1	B	593	ASN
1	B	619	THR
1	C	104	VAL
1	C	168	TRP
1	C	185	LYS
1	C	206	PHE
1	C	336	GLN
1	C	344	ASN
1	C	385	THR
1	C	389	LEU

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Mol	Chain	Res	Type
1	C	418	GLN
1	C	450	HIS
1	C	459	VAL
1	C	461	GLN
1	C	490	LYS
1	C	576	LYS
1	C	593	ASN
1	C	618	PHE
1	C	619	THR
1	D	46	LYS
1	D	82	SER
1	D	100	ILE
1	D	104	VAL
1	D	168	TRP
1	D	206	PHE
1	D	285	ARG
1	D	328	LEU
1	D	385	THR
1	D	388	GLU
1	D	389	LEU
1	D	450	HIS
1	D	459	VAL
1	D	462	SER
1	D	560	LYS
1	D	618	PHE
1	E	44	ASP
1	E	45	ILE
1	E	168	TRP
1	E	185	LYS
1	E	206	PHE
1	E	228	GLU
1	E	231	LYS
1	E	285	ARG
1	E	312	LYS
1	E	328	LEU
1	E	385	THR
1	E	388	GLU
1	E	403	LYS
1	E	450	HIS
1	E	459	VAL
1	E	618	PHE
1	F	46	LYS

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Mol	Chain	Res	Type
1	F	121	LEU
1	F	168	TRP
1	F	178	GLU
1	F	206	PHE
1	F	285	ARG
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	450	HIS
1	F	459	VAL
1	F	460	GLN
1	F	465	SER
1	F	490	LYS
1	F	546	VAL
1	F	576	LYS
1	F	618	PHE
1	G	168	TRP
1	G	206	PHE
1	G	228	GLU
1	G	272	GLU
1	G	312	LYS
1	G	385	THR
1	G	389	LEU
1	G	408	TRP
1	G	450	HIS
1	G	459	VAL
1	G	496	ASN
1	G	528	LYS
1	G	618	PHE
1	H	45	ILE
1	H	100	ILE
1	H	104	VAL
1	H	168	TRP
1	H	185	LYS
1	H	206	PHE
1	H	328	LEU
1	H	389	LEU
1	H	400	SER

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Mol	Chain	Res	Type
1	H	421	GLU
1	H	450	HIS
1	H	455	SER
1	H	460	GLN
1	H	496	ASN
1	H	560	LYS
1	H	593	ASN
1	H	618	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	HIS
1	A	341	ASN
1	A	460	GLN
1	B	336	GLN
1	B	460	GLN
1	B	611	GLN
1	C	324	HIS
1	C	341	ASN
1	C	344	ASN
1	C	418	GLN
1	C	448	GLN
1	D	263	GLN
1	D	299	HIS
1	D	324	HIS
1	D	341	ASN
1	D	460	GLN
1	E	99	ASN
1	E	324	HIS
1	E	341	ASN
1	E	418	GLN
1	E	460	GLN
1	E	611	GLN
1	F	299	HIS
1	F	324	HIS
1	F	448	GLN
1	G	263	GLN
1	G	324	HIS
1	G	418	GLN
1	G	460	GLN
1	H	110	GLN

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Mol	Chain	Res	Type
1	H	341	ASN
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 monosaccharides 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	A	801	1	53,58,58	1.46	8 (15%)	68,89,89	2.32	22 (32%)
2	FAD	F	801	1	53,58,58	1.47	10 (18%)	68,89,89	2.19	18 (26%)
2	FAD	E	801	1	53,58,58	1.15	2 (3%)	68,89,89	2.17	21 (30%)
2	FAD	H	801	1	53,58,58	1.24	3 (5%)	68,89,89	2.08	19 (27%)
2	FAD	G	801	1	53,58,58	1.41	8 (15%)	68,89,89	2.44	24 (35%)
2	FAD	D	801	1	53,58,58	1.25	10 (18%)	68,89,89	2.26	24 (35%)
2	FAD	C	801	1	53,58,58	1.42	8 (15%)	68,89,89	2.37	25 (36%)
2	FAD	B	801	1	53,58,58	1.45	9 (16%)	68,89,89	2.04	21 (30%)

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	A	801	1	-	1/30/50/50	0/6/6/6
2	FAD	F	801	1	-	3/30/50/50	0/6/6/6
2	FAD	E	801	1	-	4/30/50/50	0/6/6/6
2	FAD	H	801	1	-	2/30/50/50	0/6/6/6
2	FAD	G	801	1	-	2/30/50/50	0/6/6/6
2	FAD	D	801	1	-	2/30/50/50	0/6/6/6
2	FAD	C	801	1	-	1/30/50/50	0/6/6/6
2	FAD	B	801	1	-	2/30/50/50	0/6/6/6

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	801	FAD	C6-C5X	4.39	1.46	1.40
2	F	801	FAD	C4X-N5	4.19	1.38	1.30
2	C	801	FAD	C6-C5X	3.62	1.45	1.40
2	G	801	FAD	C10-N1	3.49	1.40	1.33
2	A	801	FAD	O2B-C2B	-3.47	1.34	1.43
2	B	801	FAD	C6-C5X	3.36	1.45	1.40
2	A	801	FAD	C2B-C3B	-3.32	1.44	1.53
2	G	801	FAD	O2B-C2B	-3.27	1.35	1.43
2	F	801	FAD	C2B-C1B	-3.19	1.48	1.53
2	A	801	FAD	C2-N3	-3.17	1.31	1.39
2	A	801	FAD	C2B-C1B	-3.10	1.49	1.53
2	B	801	FAD	C5X-N5	-3.02	1.33	1.39
2	B	801	FAD	C2B-C3B	-2.93	1.45	1.53
2	G	801	FAD	O4B-C4B	-2.85	1.38	1.45
2	B	801	FAD	C7M-C7	2.78	1.56	1.51
2	C	801	FAD	O3B-C3B	-2.74	1.36	1.43
2	A	801	FAD	C4-N3	-2.74	1.33	1.38
2	F	801	FAD	C1'-C2'	-2.71	1.48	1.52
2	F	801	FAD	O2B-C2B	-2.67	1.36	1.43
2	B	801	FAD	C2-N3	-2.66	1.32	1.39
2	G	801	FAD	C2-N3	-2.64	1.32	1.39
2	B	801	FAD	C2A-N3A	2.64	1.36	1.32
2	C	801	FAD	C2A-N3A	2.61	1.36	1.32
2	C	801	FAD	C10-N1	2.60	1.38	1.33
2	B	801	FAD	O2B-C2B	-2.59	1.36	1.43
2	F	801	FAD	C4-N3	-2.59	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FAD	C4X-N5	2.59	1.35	1.30
2	F	801	FAD	C6-C5X	2.52	1.43	1.40
2	H	801	FAD	C2-N3	-2.42	1.33	1.39
2	B	801	FAD	C4-N3	-2.41	1.34	1.38
2	F	801	FAD	C2-N3	-2.39	1.33	1.39
2	A	801	FAD	O2'-C2'	-2.38	1.38	1.43
2	D	801	FAD	C6-C5X	2.36	1.43	1.40
2	G	801	FAD	C2B-C3B	-2.34	1.46	1.53
2	C	801	FAD	O4B-C1B	2.34	1.44	1.41
2	G	801	FAD	O3B-C3B	-2.30	1.37	1.43
2	F	801	FAD	C4X-C10	-2.26	1.37	1.44
2	D	801	FAD	O3B-C3B	-2.19	1.37	1.43
2	D	801	FAD	C3B-C4B	-2.19	1.47	1.53
2	C	801	FAD	C2-N3	-2.17	1.34	1.39
2	A	801	FAD	C4'-C3'	-2.17	1.49	1.53
2	D	801	FAD	C9A-C5X	-2.15	1.37	1.41
2	D	801	FAD	C5X-N5	-2.14	1.35	1.39
2	E	801	FAD	O4'-C4'	-2.13	1.38	1.43
2	E	801	FAD	C5X-N5	-2.11	1.35	1.39
2	G	801	FAD	C4X-C10	-2.10	1.37	1.44
2	D	801	FAD	PA-O2A	-2.09	1.45	1.55
2	D	801	FAD	O5B-C5B	-2.08	1.36	1.44
2	C	801	FAD	C5X-N5	-2.08	1.35	1.39
2	B	801	FAD	O3B-C3B	-2.07	1.38	1.43
2	F	801	FAD	O3B-C3B	-2.06	1.38	1.43
2	G	801	FAD	C7M-C7	2.05	1.55	1.51
2	A	801	FAD	C4X-C10	-2.05	1.38	1.44
2	D	801	FAD	O2B-C2B	-2.03	1.38	1.43
2	D	801	FAD	C2-N3	-2.02	1.34	1.39
2	H	801	FAD	C2-N1	-2.01	1.32	1.36
2	D	801	FAD	C2B-C3B	-2.01	1.47	1.53
2	F	801	FAD	O2'-C2'	-2.00	1.39	1.43

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	C4-N3-C2	7.38	139.28	125.64
2	F	801	FAD	N3A-C2A-N1A	-7.28	117.29	128.68
2	A	801	FAD	N3A-C2A-N1A	-6.63	118.32	128.68
2	G	801	FAD	N3A-C2A-N1A	-6.50	118.52	128.68
2	C	801	FAD	N3A-C2A-N1A	-6.41	118.66	128.68
2	G	801	FAD	N3-C2-N1	-6.28	107.07	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	FAD	C4-C4X-N5	6.26	127.13	118.23
2	H	801	FAD	N3A-C2A-N1A	-6.25	118.90	128.68
2	A	801	FAD	O3B-C3B-C4B	6.05	128.53	111.05
2	G	801	FAD	C5A-C6A-N6A	5.83	129.21	120.35
2	G	801	FAD	C4-C4X-C10	-5.77	107.11	116.79
2	E	801	FAD	O4-C4-N3	5.73	131.09	120.12
2	C	801	FAD	O4-C4-C4X	-5.71	111.44	126.60
2	D	801	FAD	N3A-C2A-N1A	-5.70	119.76	128.68
2	E	801	FAD	N3A-C2A-N1A	-5.61	119.91	128.68
2	G	801	FAD	O3B-C3B-C4B	5.60	127.25	111.05
2	D	801	FAD	C9A-C5X-N5	-5.49	116.47	122.43
2	H	801	FAD	O3B-C3B-C4B	5.46	126.84	111.05
2	D	801	FAD	C5A-C6A-N6A	5.44	128.62	120.35
2	C	801	FAD	O3B-C3B-C4B	5.21	126.12	111.05
2	F	801	FAD	O4-C4-C4X	-5.12	113.01	126.60
2	H	801	FAD	O4B-C1B-C2B	5.05	114.30	106.93
2	E	801	FAD	O3B-C3B-C4B	5.04	125.63	111.05
2	E	801	FAD	O2B-C2B-C3B	5.04	128.12	111.82
2	F	801	FAD	C2A-N1A-C6A	4.96	127.23	118.75
2	B	801	FAD	O4-C4-N3	4.95	129.60	120.12
2	B	801	FAD	N3A-C2A-N1A	-4.89	121.04	128.68
2	F	801	FAD	O4-C4-N3	4.86	129.43	120.12
2	E	801	FAD	O4-C4-C4X	-4.86	113.72	126.60
2	A	801	FAD	N3-C2-N1	-4.78	110.01	119.38
2	D	801	FAD	O3B-C3B-C4B	4.72	124.69	111.05
2	C	801	FAD	C9A-C5X-N5	-4.66	117.36	122.43
2	B	801	FAD	O4-C4-C4X	-4.66	114.24	126.60
2	D	801	FAD	O4-C4-N3	4.62	128.97	120.12
2	F	801	FAD	C9A-C5X-N5	-4.59	117.44	122.43
2	A	801	FAD	C4X-C4-N3	-4.57	101.59	113.19
2	C	801	FAD	O2B-C2B-C1B	4.53	127.59	110.85
2	C	801	FAD	O4-C4-N3	4.48	128.71	120.12
2	G	801	FAD	O4-C4-C4X	-4.45	114.78	126.60
2	F	801	FAD	O3B-C3B-C4B	4.35	123.64	111.05
2	H	801	FAD	C9A-C5X-N5	-4.27	117.79	122.43
2	G	801	FAD	C10-N1-C2	4.20	125.29	116.90
2	E	801	FAD	C9A-C5X-N5	-4.18	117.89	122.43
2	H	801	FAD	C4-N3-C2	4.14	133.30	125.64
2	A	801	FAD	O4B-C1B-C2B	4.12	112.94	106.93
2	C	801	FAD	C9-C8-C7	4.02	125.42	119.67
2	A	801	FAD	O4B-C4B-C5B	4.01	122.55	109.37
2	G	801	FAD	C4-N3-C2	3.99	133.02	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	801	FAD	C5B-C4B-C3B	3.97	130.06	115.18
2	F	801	FAD	C9-C8-C7	3.97	125.35	119.67
2	H	801	FAD	O2B-C2B-C1B	3.97	125.50	110.85
2	D	801	FAD	C2A-N1A-C6A	3.83	125.31	118.75
2	E	801	FAD	O2B-C2B-C1B	3.81	124.92	110.85
2	B	801	FAD	O4B-C4B-C5B	3.79	121.83	109.37
2	H	801	FAD	O2B-C2B-C3B	3.77	124.01	111.82
2	G	801	FAD	O2-C2-N3	3.76	125.95	118.65
2	G	801	FAD	C2A-N1A-C6A	3.71	125.10	118.75
2	B	801	FAD	O2B-C2B-C1B	3.62	124.23	110.85
2	D	801	FAD	O2B-C2B-C1B	3.61	124.17	110.85
2	D	801	FAD	C4-C4X-C10	3.60	122.83	116.79
2	F	801	FAD	C4-N3-C2	3.51	132.13	125.64
2	C	801	FAD	O2B-C2B-C3B	3.46	123.03	111.82
2	A	801	FAD	O4B-C4B-C3B	3.44	111.93	105.11
2	A	801	FAD	C4-C4X-C10	3.41	122.52	116.79
2	B	801	FAD	C5X-C6-C7	-3.41	114.46	120.71
2	E	801	FAD	C2A-N1A-C6A	3.40	124.58	118.75
2	A	801	FAD	C9A-C5X-N5	-3.38	118.75	122.43
2	B	801	FAD	C8M-C8-C9	-3.38	113.25	119.49
2	B	801	FAD	C5A-C6A-N6A	3.32	125.39	120.35
2	A	801	FAD	C2A-N1A-C6A	3.27	124.35	118.75
2	D	801	FAD	C10-C4X-N5	-3.26	117.95	124.86
2	B	801	FAD	C9A-C5X-N5	-3.22	118.93	122.43
2	F	801	FAD	C5A-C6A-N6A	3.19	125.19	120.35
2	H	801	FAD	O4B-C4B-C3B	3.18	111.41	105.11
2	C	801	FAD	C5B-C4B-C3B	3.16	127.03	115.18
2	D	801	FAD	O4B-C4B-C5B	3.13	119.67	109.37
2	C	801	FAD	C5A-C6A-N6A	3.13	125.10	120.35
2	B	801	FAD	O4B-C1B-C2B	3.11	111.48	106.93
2	G	801	FAD	O2B-C2B-C3B	3.07	121.76	111.82
2	C	801	FAD	C5'-C4'-C3'	-3.04	106.34	112.20
2	B	801	FAD	C9-C8-C7	3.03	124.01	119.67
2	G	801	FAD	O4B-C4B-C5B	3.02	119.32	109.37
2	B	801	FAD	C2A-N1A-C6A	3.01	123.91	118.75
2	D	801	FAD	O4B-C4B-C3B	3.01	111.07	105.11
2	E	801	FAD	C5A-C6A-N6A	2.95	124.84	120.35
2	B	801	FAD	O3B-C3B-C4B	2.95	119.57	111.05
2	H	801	FAD	C8M-C8-C9	-2.93	114.06	119.49
2	F	801	FAD	O2B-C2B-C3B	2.91	121.24	111.82
2	A	801	FAD	O2B-C2B-C1B	2.86	121.42	110.85
2	A	801	FAD	C3B-C2B-C1B	2.86	105.28	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	FAD	O4'-C4'-C3'	2.84	116.00	109.10
2	A	801	FAD	C5A-C6A-N6A	2.83	124.66	120.35
2	G	801	FAD	C8M-C8-C9	-2.82	114.28	119.49
2	G	801	FAD	C1B-N9A-C4A	2.78	131.53	126.64
2	D	801	FAD	O2B-C2B-C3B	2.77	120.77	111.82
2	F	801	FAD	C5B-C4B-C3B	2.77	125.54	115.18
2	D	801	FAD	C3B-C2B-C1B	2.74	105.11	100.98
2	A	801	FAD	O2B-C2B-C3B	2.71	120.57	111.82
2	D	801	FAD	C4-N3-C2	2.69	130.62	125.64
2	B	801	FAD	C1B-N9A-C4A	-2.65	121.98	126.64
2	F	801	FAD	C5X-C9A-N10	2.64	120.68	117.95
2	E	801	FAD	O4B-C4B-C3B	2.64	110.34	105.11
2	D	801	FAD	O3'-C3'-C2'	-2.61	102.50	108.81
2	C	801	FAD	O2A-PA-O1A	2.60	125.08	112.24
2	H	801	FAD	O4-C4-N3	2.59	125.08	120.12
2	E	801	FAD	C5'-C4'-C3'	-2.57	107.23	112.20
2	F	801	FAD	O2B-C2B-C1B	2.57	120.33	110.85
2	C	801	FAD	C5X-N5-C4X	2.56	122.33	118.07
2	B	801	FAD	C10-C4X-N5	-2.56	119.43	124.86
2	C	801	FAD	N3-C2-N1	-2.53	114.43	119.38
2	H	801	FAD	C2A-N1A-C6A	2.49	123.01	118.75
2	C	801	FAD	C4-C4X-C10	-2.48	112.62	116.79
2	D	801	FAD	C5A-C6A-N1A	-2.48	114.73	120.35
2	G	801	FAD	C5B-C4B-C3B	2.48	124.46	115.18
2	H	801	FAD	O2A-PA-O1A	2.48	124.48	112.24
2	E	801	FAD	O2A-PA-O1A	2.47	124.43	112.24
2	F	801	FAD	C5A-C6A-N1A	-2.45	114.80	120.35
2	D	801	FAD	O2P-P-O1P	2.44	124.28	112.24
2	B	801	FAD	C4-C4X-N5	2.42	121.68	118.23
2	G	801	FAD	C5X-C6-C7	-2.42	116.27	120.71
2	D	801	FAD	C4A-C5A-N7A	-2.41	106.89	109.40
2	E	801	FAD	O3B-C3B-C2B	2.41	119.61	111.82
2	E	801	FAD	C5X-C9A-N10	2.39	120.42	117.95
2	E	801	FAD	C3B-C2B-C1B	2.39	104.57	100.98
2	H	801	FAD	O4B-C4B-C5B	2.37	117.17	109.37
2	D	801	FAD	C7M-C7-C6	2.36	123.85	119.49
2	H	801	FAD	C5'-C4'-C3'	-2.36	107.65	112.20
2	G	801	FAD	O2B-C2B-C1B	2.35	119.53	110.85
2	F	801	FAD	O2A-PA-O1A	2.35	123.84	112.24
2	D	801	FAD	C4X-C4-N3	-2.35	107.24	113.19
2	C	801	FAD	C2A-N1A-C6A	2.34	122.76	118.75
2	C	801	FAD	C3B-C2B-C1B	2.34	104.50	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	801	FAD	C5B-C4B-C3B	2.34	123.93	115.18
2	G	801	FAD	C4-C4X-N5	2.33	121.54	118.23
2	F	801	FAD	N3-C2-N1	-2.32	114.83	119.38
2	A	801	FAD	C10-N1-C2	2.32	121.54	116.90
2	H	801	FAD	C9-C8-C7	2.31	122.97	119.67
2	B	801	FAD	C8M-C8-C7	-2.30	116.02	120.74
2	C	801	FAD	C4-N3-C2	2.29	129.88	125.64
2	H	801	FAD	O2-C2-N3	2.26	123.03	118.65
2	B	801	FAD	C4A-C5A-N7A	-2.24	107.06	109.40
2	C	801	FAD	O4'-C4'-C3'	2.24	114.54	109.10
2	E	801	FAD	C8M-C8-C7	-2.23	116.16	120.74
2	C	801	FAD	C6-C5X-C9A	2.23	122.09	118.94
2	D	801	FAD	O5'-P-O1P	-2.22	100.39	109.07
2	C	801	FAD	C10-C4X-N5	-2.19	120.20	124.86
2	A	801	FAD	O2-C2-N3	2.19	122.90	118.65
2	A	801	FAD	C9-C8-C7	2.17	122.78	119.67
2	B	801	FAD	C5B-C4B-C3B	2.17	123.32	115.18
2	C	801	FAD	C8M-C8-C9	-2.17	115.48	119.49
2	A	801	FAD	C5X-N5-C4X	2.16	121.66	118.07
2	D	801	FAD	C5X-N5-C4X	2.15	121.65	118.07
2	D	801	FAD	O2'-C2'-C1'	2.13	114.96	109.80
2	G	801	FAD	O4B-C4B-C3B	2.13	109.33	105.11
2	F	801	FAD	C3B-C2B-C1B	2.13	104.18	100.98
2	F	801	FAD	O3B-C3B-C2B	2.12	118.69	111.82
2	B	801	FAD	O2'-C2'-C3'	2.12	114.24	109.10
2	C	801	FAD	C9A-C9-C8	-2.11	115.06	119.30
2	E	801	FAD	C5A-C6A-N1A	-2.11	115.58	120.35
2	C	801	FAD	C5X-C6-C7	-2.10	116.86	120.71
2	A	801	FAD	O5'-P-O1P	-2.09	100.89	109.07
2	E	801	FAD	C6-C5X-C9A	-2.09	115.98	118.94
2	G	801	FAD	O4'-C4'-C3'	2.09	114.18	109.10
2	G	801	FAD	C5X-N5-C4X	2.08	121.53	118.07
2	E	801	FAD	O5B-C5B-C4B	2.06	116.07	108.99
2	G	801	FAD	C9A-C5X-N5	-2.05	120.20	122.43
2	H	801	FAD	N3-C2-N1	-2.05	115.35	119.38
2	G	801	FAD	C5A-C6A-N1A	-2.05	115.70	120.35
2	E	801	FAD	O2P-P-O1P	2.05	122.39	112.24
2	B	801	FAD	O2B-C2B-C3B	2.05	118.45	111.82
2	G	801	FAD	C1'-N10-C9A	2.03	123.89	120.51
2	D	801	FAD	C8M-C8-C9	-2.01	115.77	119.49
2	A	801	FAD	C4X-C10-N1	-2.01	120.07	124.73
2	A	801	FAD	C5X-C6-C7	-2.01	117.03	120.71

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

There are no ring outliers.
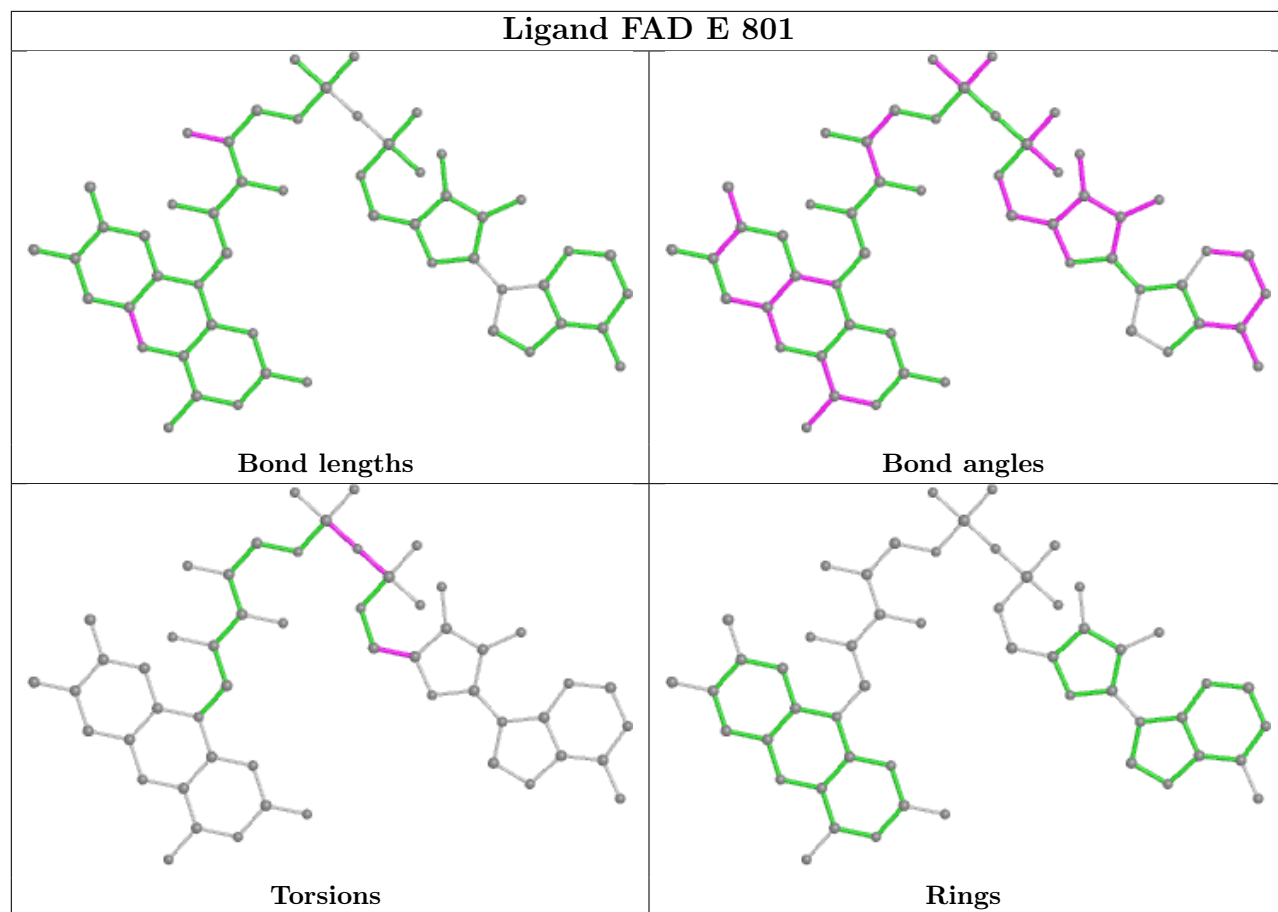
8 monomers are involved in 60 short contacts:

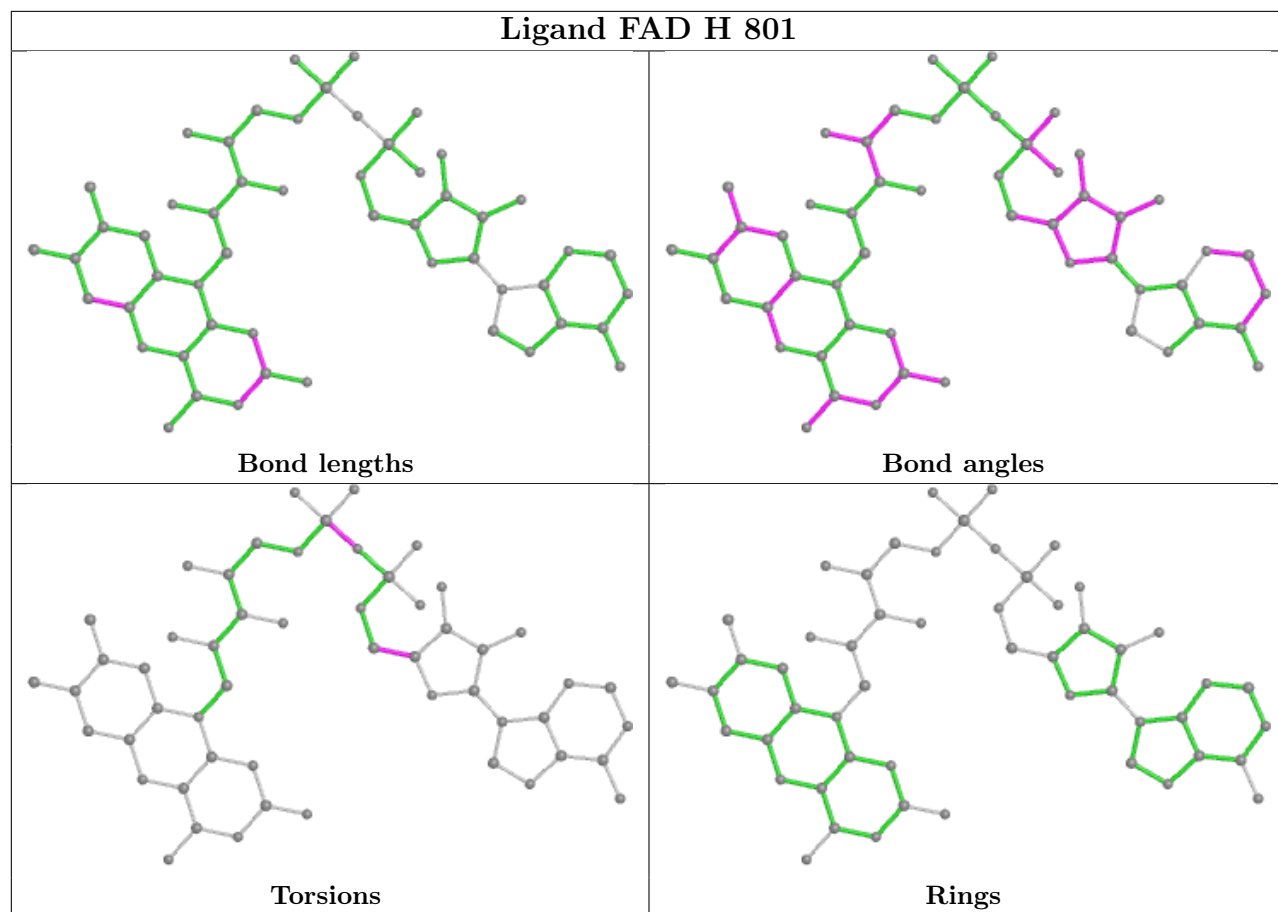| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	6	0
2	F	801	FAD	5	0
2	E	801	FAD	8	0
2	H	801	FAD	5	0
2	G	801	FAD	9	0
2	D	801	FAD	8	0
2	C	801	FAD	5	0
2	B	801	FAD	14	0

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

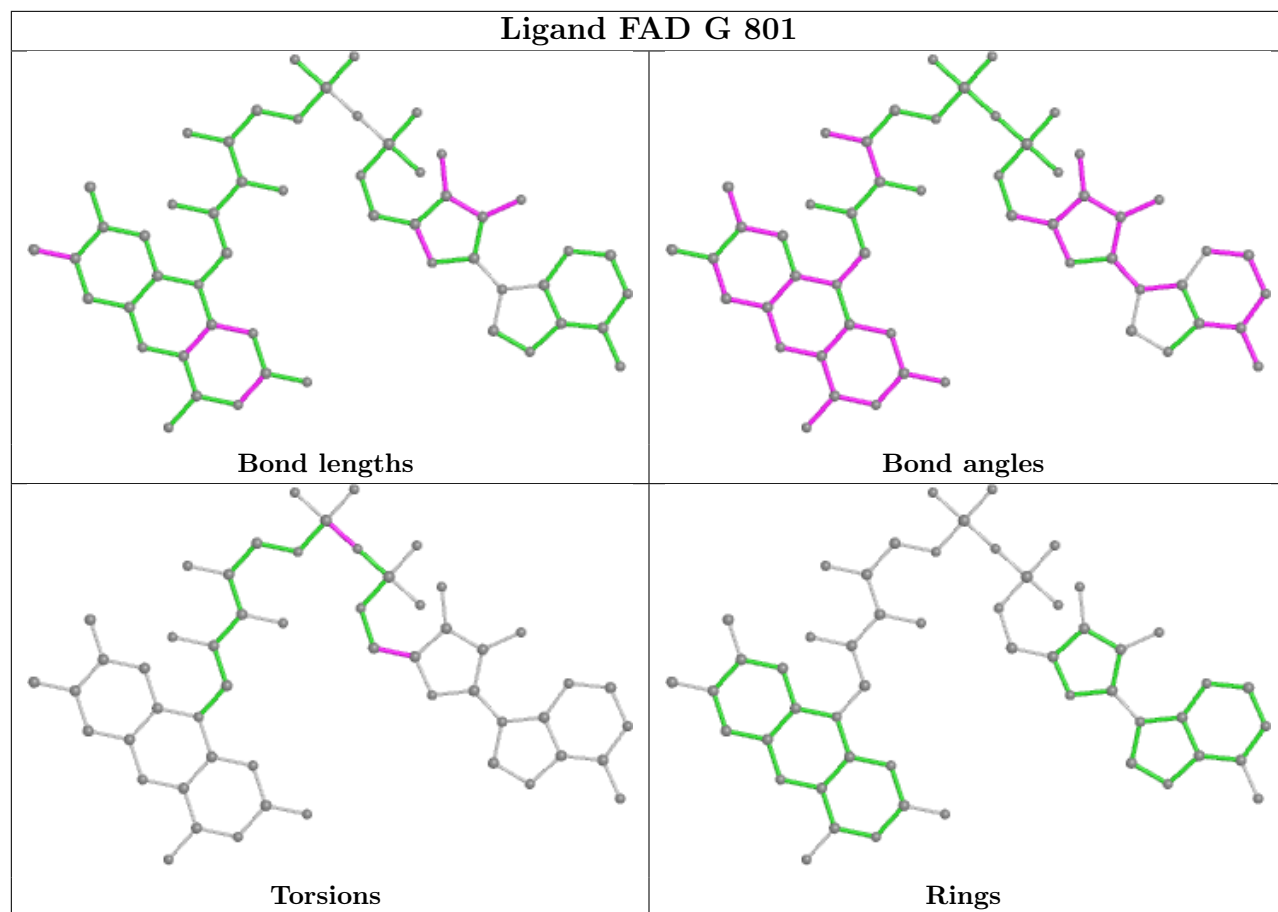any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FAD A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD F 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD E 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD H 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD G 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 801
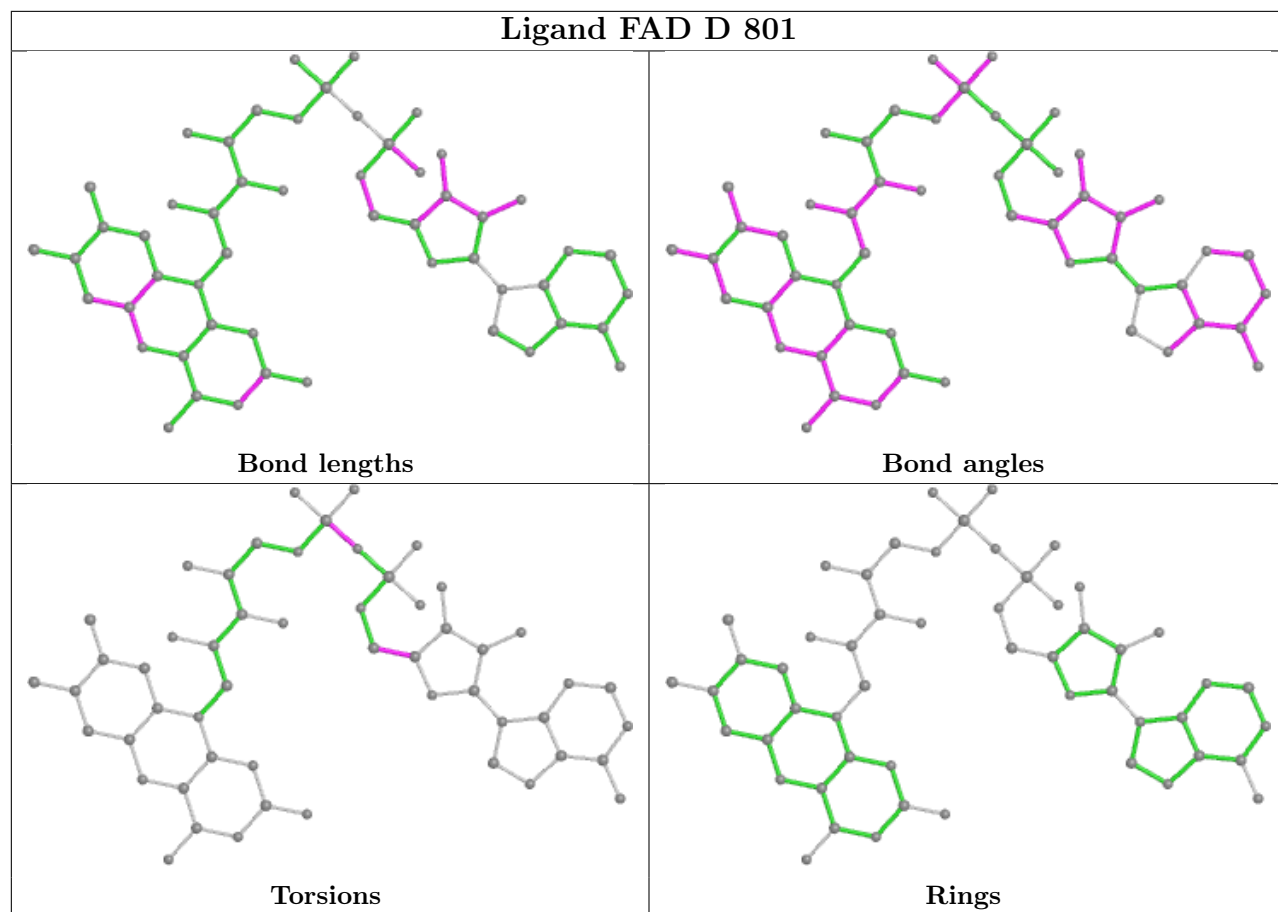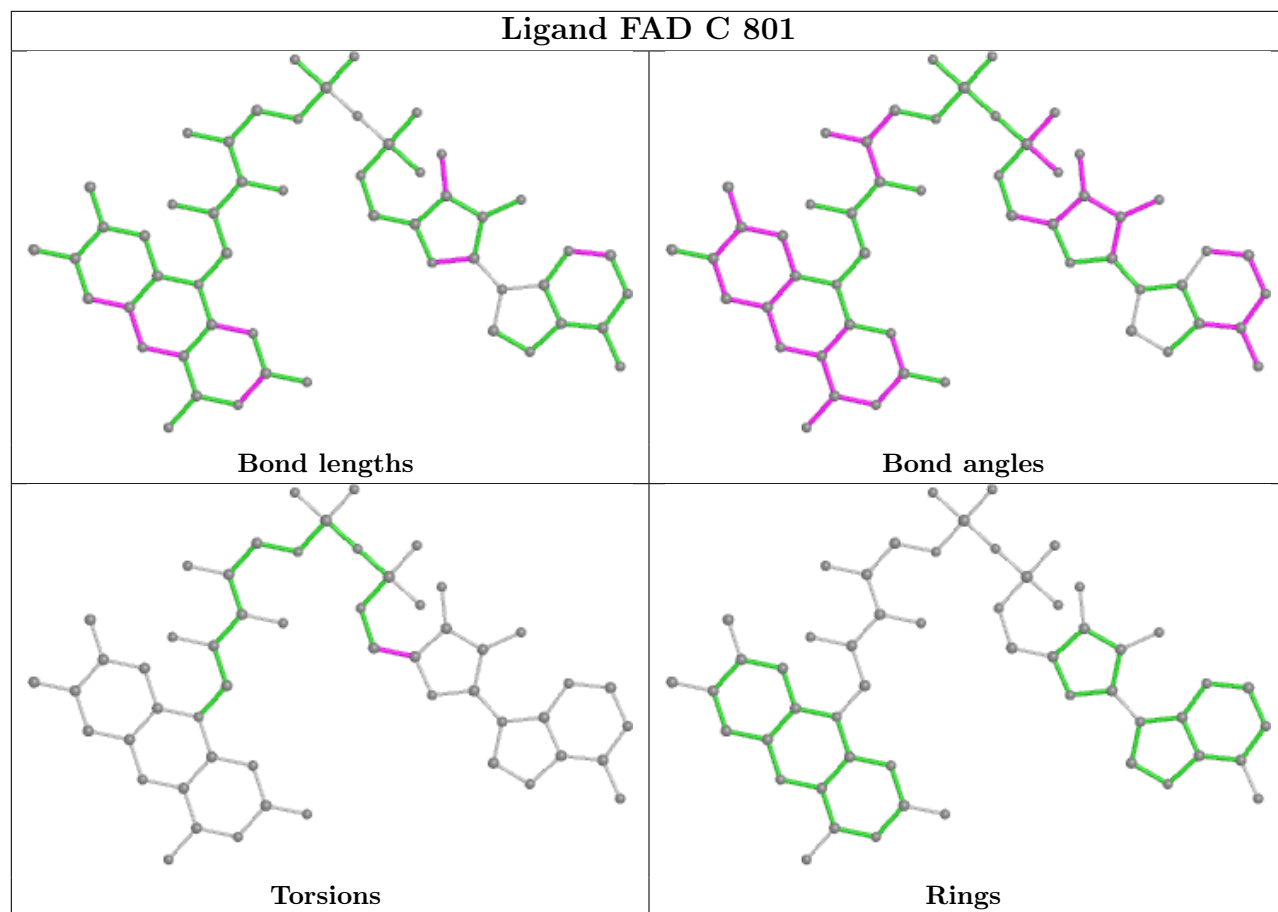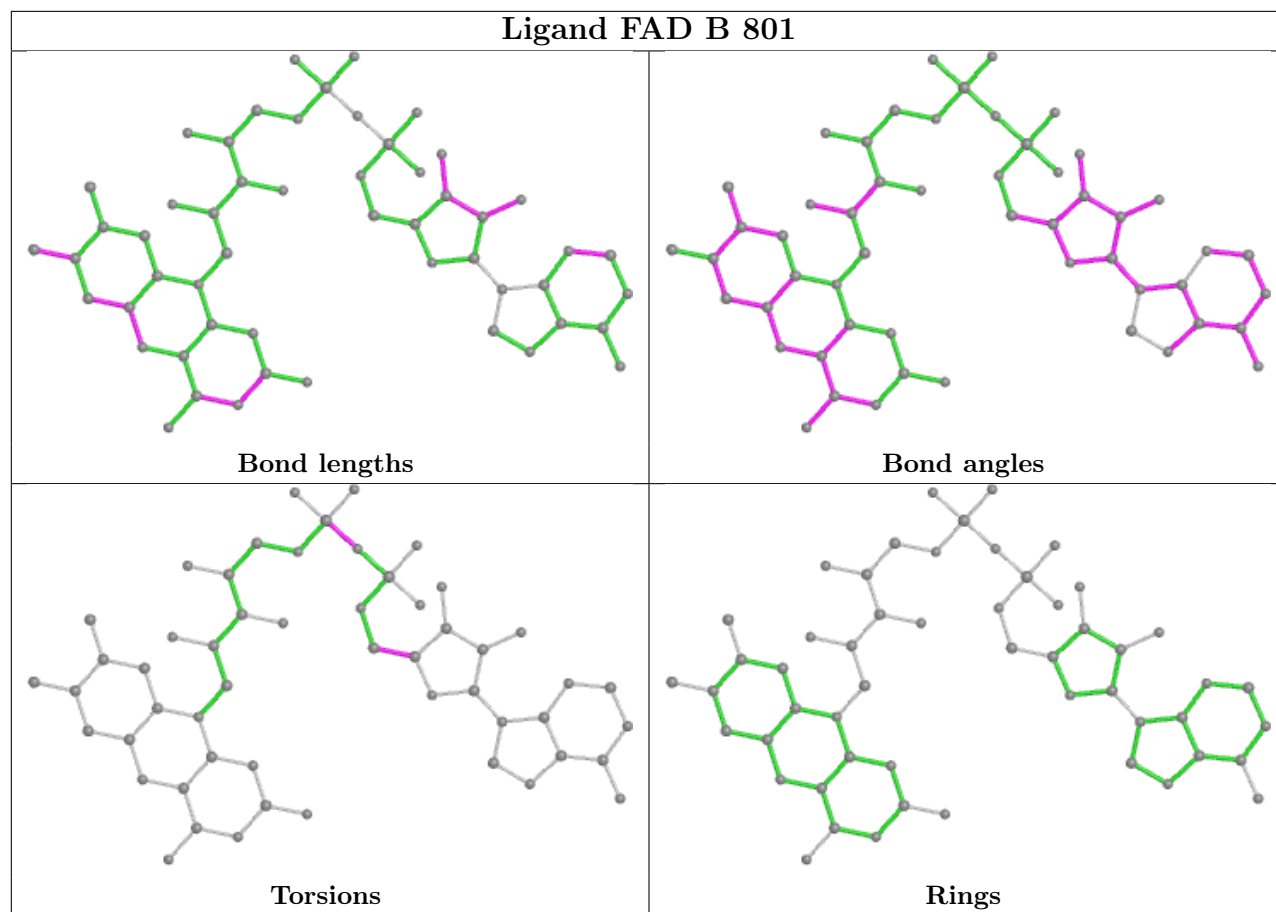

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.82	69 (11%)	4	5	20, 32, 56, 75	1 (0%)
1	B	577/623 (92%)	0.82	62 (10%)	6	7	19, 33, 54, 77	2 (0%)
1	C	577/623 (92%)	0.94	81 (14%)	2	3	22, 38, 57, 83	2 (0%)
1	D	577/623 (92%)	0.93	77 (13%)	3	4	24, 36, 57, 77	2 (0%)
1	E	577/623 (92%)	1.02	97 (16%)	1	2	25, 39, 59, 81	2 (0%)
1	F	577/623 (92%)	1.00	96 (16%)	1	2	26, 40, 59, 83	1 (0%)
1	G	577/623 (92%)	0.87	81 (14%)	2	3	23, 36, 56, 78	3 (0%)
1	H	577/623 (92%)	0.80	68 (11%)	4	5	22, 35, 53, 78	3 (0%)
All	All	4616/4984 (92%)	0.90	631 (13%)	3	4	19, 36, 57, 83	16 (0%)

All (631) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	619	THR	12.2
1	G	619	THR	11.6
1	C	619	THR	11.0
1	H	619	THR	10.4
1	D	619	THR	10.1
1	A	619	THR	10.1
1	B	459	VAL	9.8
1	A	343	ALA	9.6
1	F	459	VAL	8.9
1	A	385	THR	8.6
1	B	343	ALA	8.6
1	F	343	ALA	8.6
1	E	619	THR	8.2
1	D	344	ASN	7.9
1	G	389	LEU	7.6
1	E	385	THR	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	459	VAL	7.5
1	F	619	THR	7.5
1	C	343	ALA	7.4
1	E	459	VAL	7.3
1	C	459	VAL	7.3
1	E	44	ASP	7.1
1	F	43	MET	7.0
1	C	385	THR	7.0
1	H	343	ALA	6.9
1	G	43	MET	6.9
1	F	44	ASP	6.9
1	F	342	PRO	6.9
1	B	44	ASP	6.8
1	D	343	ALA	6.8
1	D	43	MET	6.8
1	A	458	ALA	6.7
1	H	132	GLN	6.7
1	B	43	MET	6.7
1	C	389	LEU	6.6
1	C	43	MET	6.5
1	E	389	LEU	6.5
1	F	232	GLY	6.5
1	F	345	PRO	6.4
1	G	186	ASP	6.4
1	D	345	PRO	6.4
1	C	384	GLY	6.3
1	G	388	GLU	6.3
1	E	618	PHE	6.3
1	B	385	THR	6.3
1	E	342	PRO	6.2
1	G	343	ALA	6.2
1	B	389	LEU	6.2
1	F	344	ASN	6.2
1	H	344	ASN	6.2
1	A	43	MET	6.2
1	D	458	ALA	6.1
1	D	45	ILE	6.0
1	D	132	GLN	6.0
1	E	43	MET	6.0
1	G	44	ASP	5.9
1	D	459	VAL	5.9
1	E	132	GLN	5.9

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Mol	Chain	Res	Type	RSRZ
1	H	43	MET	5.8
1	C	618	PHE	5.8
1	C	344	ASN	5.8
1	G	345	PRO	5.8
1	E	45	ILE	5.8
1	A	384	GLY	5.7
1	G	385	THR	5.6
1	H	44	ASP	5.6
1	B	186	ASP	5.5
1	E	344	ASN	5.4
1	B	458	ALA	5.4
1	E	458	ALA	5.4
1	H	342	PRO	5.4
1	E	455	SER	5.4
1	H	186	ASP	5.4
1	F	454	PHE	5.3
1	B	456	TYR	5.3
1	C	44	ASP	5.3
1	F	455	SER	5.3
1	F	385	THR	5.3
1	C	132	GLN	5.3
1	A	388	GLU	5.3
1	A	383	ARG	5.3
1	H	45	ILE	5.3
1	F	187	ASP	5.2
1	A	390	THR	5.2
1	B	344	ASN	5.2
1	D	389	LEU	5.1
1	E	384	GLY	5.1
1	H	617	PRO	5.1
1	D	186	ASP	5.1
1	D	388	GLU	5.1
1	A	186	ASP	5.1
1	G	299	HIS	5.0
1	F	341	ASN	5.0
1	G	132	GLN	5.0
1	E	57	ILE	5.0
1	H	618	PHE	4.9
1	C	342	PRO	4.9
1	B	454	PHE	4.9
1	C	383	ARG	4.8
1	D	385	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	401	THR	4.8
1	C	186	ASP	4.7
1	G	45	ILE	4.7
1	C	341	ASN	4.7
1	E	186	ASP	4.6
1	C	51	ILE	4.6
1	C	388	GLU	4.6
1	A	406	ASP	4.6
1	A	344	ASN	4.6
1	G	344	ASN	4.6
1	D	549	LEU	4.5
1	H	57	ILE	4.5
1	E	617	PRO	4.5
1	G	382	ILE	4.5
1	G	268	THR	4.5
1	E	549	LEU	4.5
1	E	388	GLU	4.5
1	G	618	PHE	4.5
1	E	184	VAL	4.5
1	F	546	VAL	4.5
1	H	341	ASN	4.5
1	B	45	ILE	4.4
1	A	44	ASP	4.4
1	E	400	SER	4.4
1	E	456	TYR	4.4
1	D	382	ILE	4.4
1	A	386	PRO	4.4
1	D	44	ASP	4.4
1	E	306	GLY	4.4
1	D	269	ASP	4.4
1	G	455	SER	4.4
1	G	188	ALA	4.3
1	D	454	PHE	4.3
1	F	290	ALA	4.3
1	G	459	VAL	4.3
1	C	57	ILE	4.3
1	A	549	LEU	4.3
1	C	456	TYR	4.3
1	C	268	THR	4.3
1	F	388	GLU	4.2
1	F	387	GLY	4.2
1	C	45	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	188	ALA	4.2
1	A	381	THR	4.2
1	A	389	LEU	4.2
1	E	318	LEU	4.2
1	A	456	TYR	4.2
1	F	189	ASP	4.1
1	E	320	ALA	4.1
1	D	268	THR	4.1
1	F	186	ASP	4.1
1	B	132	GLN	4.1
1	H	456	TYR	4.1
1	C	390	THR	4.1
1	D	232	GLY	4.0
1	B	187	ASP	4.0
1	G	187	ASP	4.0
1	E	271	PRO	4.0
1	G	456	TYR	4.0
1	E	341	ASN	4.0
1	H	458	ALA	4.0
1	G	57	ILE	4.0
1	C	272	GLU	4.0
1	A	57	ILE	3.9
1	E	187	ASP	3.9
1	G	454	PHE	3.9
1	H	189	ASP	3.9
1	E	268	THR	3.9
1	H	345	PRO	3.8
1	C	455	SER	3.8
1	D	187	ASP	3.8
1	G	421	GLU	3.8
1	E	547	LEU	3.8
1	G	549	LEU	3.8
1	H	549	LEU	3.8
1	D	401	THR	3.8
1	A	317	VAL	3.8
1	G	401	THR	3.8
1	B	345	PRO	3.8
1	E	269	ASP	3.8
1	C	52	VAL	3.8
1	A	341	ASN	3.8
1	D	189	ASP	3.8
1	C	184	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	305	SER	3.8
1	F	45	ILE	3.7
1	E	561	GLU	3.7
1	H	400	SER	3.7
1	D	618	PHE	3.7
1	F	268	THR	3.7
1	F	383	ARG	3.7
1	H	271	PRO	3.7
1	C	189	ASP	3.7
1	A	345	PRO	3.7
1	C	458	ALA	3.7
1	E	189	ASP	3.7
1	F	384	GLY	3.7
1	B	390	THR	3.7
1	G	309	PHE	3.7
1	F	347	GLU	3.6
1	C	345	PRO	3.6
1	E	343	ALA	3.6
1	H	417	MET	3.6
1	E	390	THR	3.6
1	B	341	ASN	3.6
1	C	305	SER	3.6
1	G	387	GLY	3.6
1	G	400	SER	3.6
1	H	104	VAL	3.6
1	G	386	PRO	3.6
1	F	269	ASP	3.5
1	C	317	VAL	3.5
1	A	318	LEU	3.5
1	A	342	PRO	3.5
1	D	188	ALA	3.5
1	F	458	ALA	3.5
1	F	101	ASP	3.5
1	C	400	SER	3.5
1	B	52	VAL	3.5
1	E	99	ASN	3.5
1	B	51	ILE	3.5
1	E	272	GLU	3.5
1	B	387	GLY	3.5
1	A	561	GLU	3.4
1	E	329	LEU	3.4
1	G	342	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	347	GLU	3.4
1	F	586	ILE	3.4
1	A	51	ILE	3.4
1	B	549	LEU	3.4
1	H	187	ASP	3.4
1	H	561	GLU	3.4
1	F	299	HIS	3.3
1	H	268	THR	3.3
1	D	317	VAL	3.3
1	A	391	TYR	3.3
1	D	272	GLU	3.3
1	E	545	LEU	3.3
1	H	389	LEU	3.3
1	E	345	PRO	3.3
1	G	453	ALA	3.3
1	H	454	PHE	3.3
1	C	318	LEU	3.3
1	E	601	LEU	3.3
1	F	549	LEU	3.3
1	E	104	VAL	3.3
1	H	320	ALA	3.3
1	D	270	ALA	3.3
1	G	458	ALA	3.3
1	C	232	GLY	3.2
1	E	581	GLY	3.2
1	G	384	GLY	3.2
1	G	383	ARG	3.2
1	G	100	ILE	3.2
1	G	341	ASN	3.2
1	D	407	TRP	3.2
1	E	454	PHE	3.2
1	F	51	ILE	3.2
1	F	104	VAL	3.2
1	D	319	THR	3.2
1	G	52	VAL	3.2
1	A	319	THR	3.2
1	B	383	ARG	3.2
1	E	56	PRO	3.1
1	F	340	PRO	3.1
1	D	400	SER	3.1
1	F	81	ASP	3.1
1	D	320	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	389	LEU	3.1
1	E	52	VAL	3.1
1	F	192	ASP	3.1
1	F	550	GLY	3.1
1	B	57	ILE	3.1
1	B	388	GLU	3.1
1	B	392	SER	3.1
1	D	561	GLU	3.1
1	B	342	PRO	3.1
1	D	456	TYR	3.1
1	E	305	SER	3.1
1	G	317	VAL	3.1
1	F	421	GLU	3.1
1	C	583	CYS	3.1
1	F	401	THR	3.1
1	E	299	HIS	3.1
1	H	185	LYS	3.1
1	F	272	GLU	3.0
1	E	583	CYS	3.0
1	G	583	CYS	3.0
1	B	546	VAL	3.0
1	B	618	PHE	3.0
1	D	387	GLY	3.0
1	E	317	VAL	3.0
1	F	317	VAL	3.0
1	G	398	GLY	3.0
1	E	490	LYS	3.0
1	H	321	GLY	3.0
1	C	190	ALA	3.0
1	C	617	PRO	3.0
1	H	121	LEU	3.0
1	E	322	ALA	3.0
1	H	322	ALA	3.0
1	D	583	CYS	3.0
1	B	231	LYS	3.0
1	C	322	ALA	3.0
1	C	356	ILE	3.0
1	A	189	ASP	3.0
1	C	561	GLU	3.0
1	B	580	LEU	3.0
1	G	320	ALA	3.0
1	E	383	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	104	VAL	2.9
1	A	581	GLY	2.9
1	D	396	THR	2.9
1	G	323	VAL	2.9
1	H	546	VAL	2.9
1	E	325	ASN	2.9
1	E	616	SER	2.9
1	C	187	ASP	2.9
1	G	390	THR	2.9
1	H	319	THR	2.9
1	A	272	GLU	2.9
1	B	232	GLY	2.9
1	B	582	GLY	2.9
1	F	319	THR	2.9
1	D	104	VAL	2.9
1	H	323	VAL	2.9
1	E	304	ILE	2.9
1	H	53	GLY	2.9
1	C	347	GLU	2.9
1	D	560	LYS	2.9
1	E	421	GLU	2.9
1	C	323	VAL	2.8
1	E	51	ILE	2.8
1	F	57	ILE	2.8
1	A	269	ASP	2.8
1	F	191	ASP	2.8
1	G	305	SER	2.8
1	A	580	LEU	2.8
1	H	340	PRO	2.8
1	B	583	CYS	2.8
1	D	299	HIS	2.8
1	H	583	CYS	2.8
1	G	82	SER	2.8
1	G	391	TYR	2.8
1	B	318	LEU	2.8
1	E	182	LEU	2.8
1	A	347	GLU	2.8
1	A	320	ALA	2.8
1	A	382	ILE	2.8
1	F	322	ALA	2.8
1	A	421	GLU	2.8
1	D	318	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	469	VAL	2.8
1	F	508	ALA	2.8
1	B	319	THR	2.8
1	D	581	GLY	2.8
1	D	399	ALA	2.8
1	G	322	ALA	2.8
1	H	459	VAL	2.8
1	C	271	PRO	2.8
1	F	233	GLN	2.8
1	A	455	SER	2.8
1	C	401	THR	2.7
1	E	401	THR	2.7
1	C	53	GLY	2.7
1	D	391	TYR	2.7
1	D	322	ALA	2.7
1	C	104	VAL	2.7
1	F	309	PHE	2.7
1	G	321	GLY	2.7
1	G	51	ILE	2.7
1	G	558	ASP	2.7
1	C	309	PHE	2.7
1	D	342	PRO	2.7
1	F	346	PRO	2.7
1	C	580	LEU	2.7
1	D	558	ASP	2.7
1	F	490	LYS	2.7
1	H	272	GLU	2.7
1	C	307	ASP	2.7
1	D	381	THR	2.7
1	C	550	GLY	2.7
1	C	406	ASP	2.7
1	E	307	ASP	2.7
1	G	318	LEU	2.7
1	F	61	TYR	2.6
1	G	232	GLY	2.6
1	C	549	LEU	2.6
1	A	161	VAL	2.6
1	E	323	VAL	2.6
1	H	584	GLY	2.6
1	G	582	GLY	2.6
1	A	546	VAL	2.6
1	F	456	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	52	VAL	2.6
1	B	455	SER	2.6
1	C	396	THR	2.6
1	D	390	THR	2.6
1	G	319	THR	2.6
1	C	82	SER	2.6
1	F	100	ILE	2.6
1	F	249	THR	2.6
1	F	390	THR	2.6
1	F	561	GLU	2.6
1	D	582	GLY	2.6
1	C	547	LEU	2.6
1	E	580	LEU	2.6
1	C	392	SER	2.6
1	E	319	THR	2.6
1	F	382	ILE	2.6
1	E	347	GLU	2.6
1	F	231	LYS	2.5
1	B	317	VAL	2.5
1	E	469	VAL	2.5
1	D	305	SER	2.5
1	E	598	ALA	2.5
1	C	407	TRP	2.5
1	H	560	LYS	2.5
1	E	467	LEU	2.5
1	A	400	SER	2.5
1	A	104	VAL	2.5
1	B	188	ALA	2.5
1	A	398	GLY	2.5
1	E	61	TYR	2.5
1	D	617	PRO	2.5
1	H	307	ASP	2.5
1	A	618	PHE	2.5
1	E	298	LEU	2.5
1	H	318	LEU	2.5
1	A	270	ALA	2.5
1	H	387	GLY	2.5
1	F	391	TYR	2.5
1	C	267	ASN	2.5
1	F	321	GLY	2.5
1	F	320	ALA	2.5
1	H	388	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	460	GLN	2.5
1	B	58	GLY	2.5
1	E	560	LYS	2.5
1	G	469	VAL	2.5
1	H	469	VAL	2.5
1	F	325	ASN	2.5
1	D	51	ILE	2.5
1	H	582	GLY	2.5
1	H	190	ALA	2.5
1	G	580	LEU	2.4
1	E	496	ASN	2.4
1	B	561	GLU	2.4
1	F	452	ASP	2.4
1	A	584	GLY	2.4
1	G	551	GLY	2.4
1	D	57	ILE	2.4
1	F	474	PHE	2.4
1	C	467	LEU	2.4
1	F	291	LEU	2.4
1	H	191	ASP	2.4
1	F	184	VAL	2.4
1	D	321	GLY	2.4
1	D	347	GLU	2.4
1	E	386	PRO	2.4
1	G	617	PRO	2.4
1	H	267	ASN	2.4
1	E	558	ASP	2.4
1	D	586	ILE	2.4
1	E	594	PRO	2.4
1	H	356	ILE	2.4
1	C	551	GLY	2.4
1	F	581	GLY	2.4
1	G	561	GLU	2.4
1	F	307	ASP	2.4
1	A	188	ALA	2.4
1	C	320	ALA	2.4
1	C	319	THR	2.4
1	G	586	ILE	2.4
1	A	58	GLY	2.4
1	A	321	GLY	2.4
1	E	53	GLY	2.4
1	D	59	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	250	PHE	2.4
1	F	329	LEU	2.4
1	D	341	ASN	2.4
1	G	269	ASP	2.4
1	F	618	PHE	2.3
1	H	474	PHE	2.3
1	D	194	GLU	2.3
1	C	72	VAL	2.3
1	D	546	VAL	2.3
1	C	340	PRO	2.3
1	D	271	PRO	2.3
1	F	266	PRO	2.3
1	F	442	SER	2.3
1	G	508	ALA	2.3
1	B	468	ILE	2.3
1	A	454	PHE	2.3
1	F	547	LEU	2.3
1	E	58	GLY	2.3
1	F	55	GLY	2.3
1	A	249	THR	2.3
1	G	233	GLN	2.3
1	B	594	PRO	2.3
1	H	580	LEU	2.3
1	D	163	GLY	2.3
1	D	457	GLY	2.3
1	E	232	GLY	2.3
1	D	490	LYS	2.3
1	G	403	LYS	2.3
1	F	271	PRO	2.3
1	E	582	GLY	2.3
1	F	318	LEU	2.3
1	B	228	GLU	2.3
1	F	583	CYS	2.3
1	G	550	GLY	2.3
1	H	457	GLY	2.3
1	F	580	LEU	2.3
1	B	322	ALA	2.3
1	B	161	VAL	2.3
1	E	54	SER	2.3
1	E	266	PRO	2.3
1	A	582	GLY	2.3
1	B	321	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	382	ILE	2.3
1	F	86	ILE	2.3
1	B	545	LEU	2.2
1	D	598	ALA	2.2
1	G	121	LEU	2.2
1	F	381	THR	2.2
1	A	52	VAL	2.2
1	E	418	GLN	2.2
1	A	387	GLY	2.2
1	B	59	CYS	2.2
1	C	231	LYS	2.2
1	D	356	ILE	2.2
1	F	447	THR	2.2
1	G	467	LEU	2.2
1	D	66	VAL	2.2
1	A	53	GLY	2.2
1	C	321	GLY	2.2
1	E	248	PRO	2.2
1	F	551	GLY	2.2
1	H	56	PRO	2.2
1	H	467	LEU	2.2
1	A	56	PRO	2.2
1	C	387	GLY	2.2
1	E	550	GLY	2.2
1	E	579	PHE	2.2
1	C	558	ASP	2.2
1	G	270	ALA	2.2
1	H	455	SER	2.2
1	H	269	ASP	2.2
1	D	256	ALA	2.2
1	F	168	TRP	2.2
1	G	307	ASP	2.2
1	D	65	LEU	2.2
1	B	307	ASP	2.2
1	C	193	ALA	2.2
1	E	101	ASP	2.2
1	E	321	GLY	2.2
1	F	270	ALA	2.2
1	B	490	LYS	2.2
1	H	51	ILE	2.1
1	F	374	ASP	2.1
1	B	270	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	551	GLY	2.1
1	G	381	THR	2.1
1	A	121	LEU	2.1
1	B	329	LEU	2.1
1	E	196	ASP	2.1
1	B	306	GLY	2.1
1	B	550	GLY	2.1
1	B	581	GLY	2.1
1	F	162	GLY	2.1
1	C	598	ALA	2.1
1	C	397	PRO	2.1
1	F	352	LEU	2.1
1	B	384	GLY	2.1
1	C	546	VAL	2.1
1	D	435	VAL	2.1
1	C	248	PRO	2.1
1	A	548	HIS	2.1
1	C	58	GLY	2.1
1	A	392	SER	2.1
1	G	546	VAL	2.1
1	A	617	PRO	2.1
1	B	453	ALA	2.1
1	C	454	PHE	2.1
1	G	271	PRO	2.1
1	E	381	THR	2.1
1	E	339	ARG	2.1
1	G	452	ASP	2.1
1	A	232	GLY	2.1
1	C	581	GLY	2.1
1	E	387	GLY	2.1
1	H	550	GLY	2.1
1	G	449	ILE	2.1
1	B	315	VAL	2.1
1	E	161	VAL	2.1
1	F	367	VAL	2.1
1	G	347	GLU	2.1
1	H	317	VAL	2.1
1	F	598	ALA	2.1
1	G	62	ALA	2.1
1	E	553	HIS	2.1
1	A	550	GLY	2.1
1	G	58	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	397	PRO	2.0
1	C	601	LEU	2.0
1	F	562	ASP	2.0
1	A	602	ALA	2.0
1	D	52	VAL	2.0
1	D	286	VAL	2.0
1	H	435	VAL	2.0
1	E	478	GLU	2.0
1	A	449	ILE	2.0
1	C	121	LEU	2.0
1	E	190	ALA	2.0
1	F	62	ALA	2.0
1	H	60	THR	2.0
1	B	367	VAL	2.0
1	D	58	GLY	2.0
1	A	307	ASP	2.0
1	F	386	PRO	2.0
1	C	228	GLU	2.0
1	D	580	LEU	2.0
1	G	399	ALA	2.0
1	B	418	GLN	2.0
1	C	490	LYS	2.0
1	D	469	VAL	2.0
1	F	108	GLN	2.0
1	F	582	GLY	2.0
1	G	53	GLY	2.0
1	G	306	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	E	801	53/53	0.92	0.19	21,30,35,38	0
2	FAD	G	801	53/53	0.92	0.22	20,24,30,33	0
2	FAD	F	801	53/53	0.93	0.20	16,28,33,35	0
2	FAD	C	801	53/53	0.93	0.18	23,29,35,43	0
2	FAD	H	801	53/53	0.94	0.21	19,27,31,32	0
2	FAD	A	801	53/53	0.95	0.19	20,24,30,35	0
2	FAD	D	801	53/53	0.95	0.22	23,27,31,35	0
2	FAD	B	801	53/53	0.95	0.17	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 E 801:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
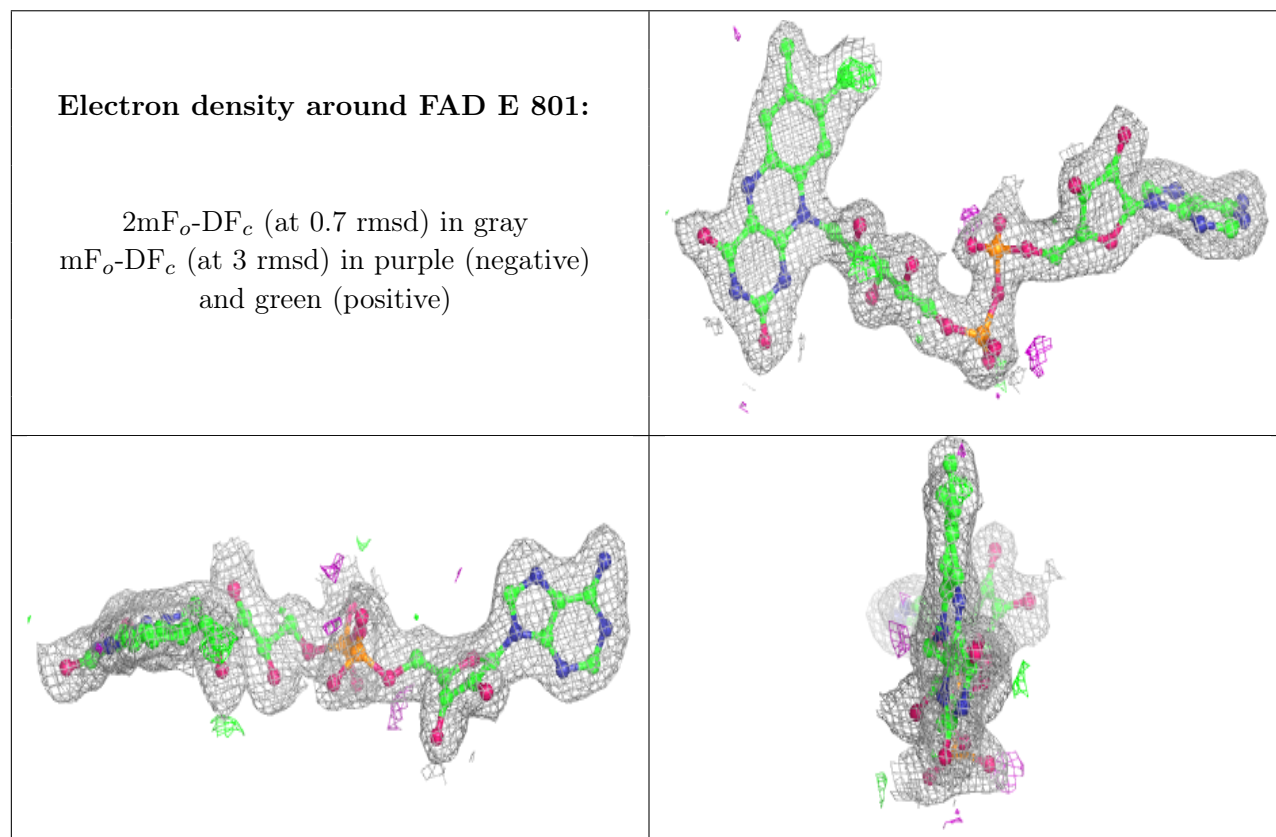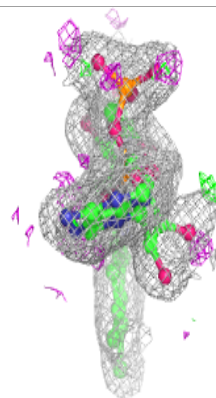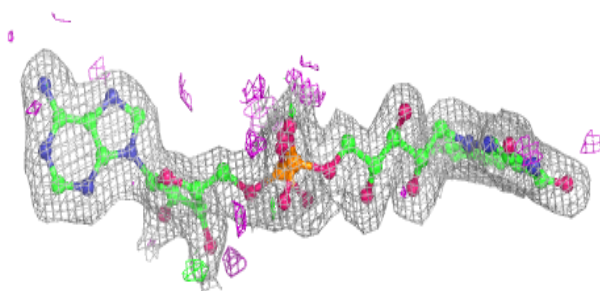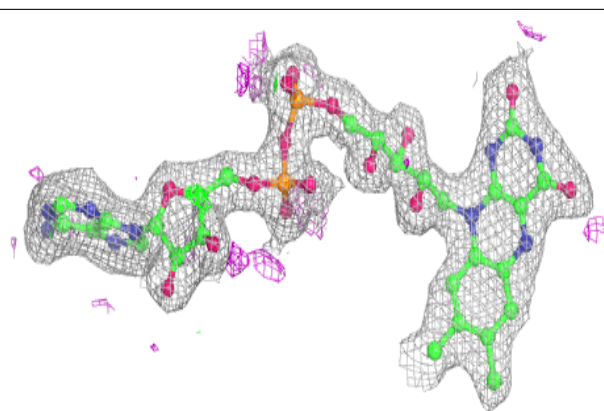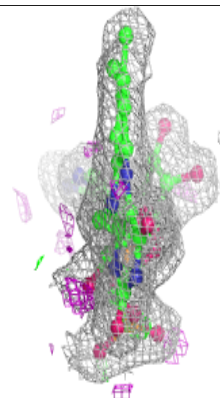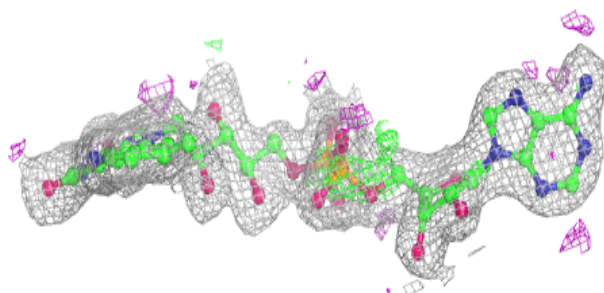
Electron density around FAD G 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
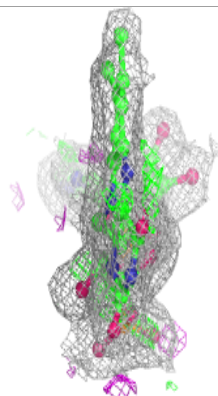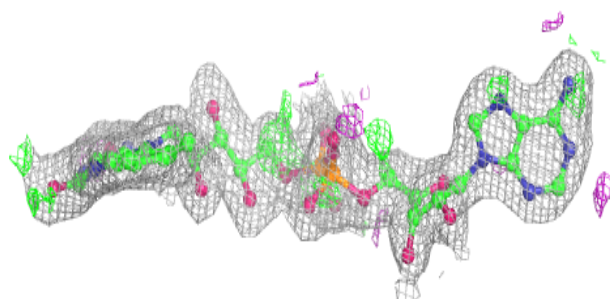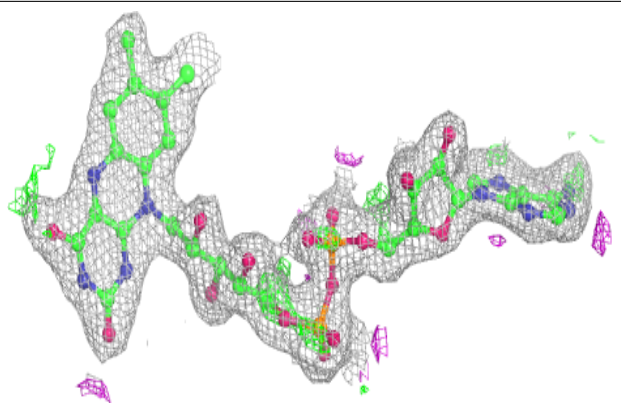
Electron density around FAD F 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
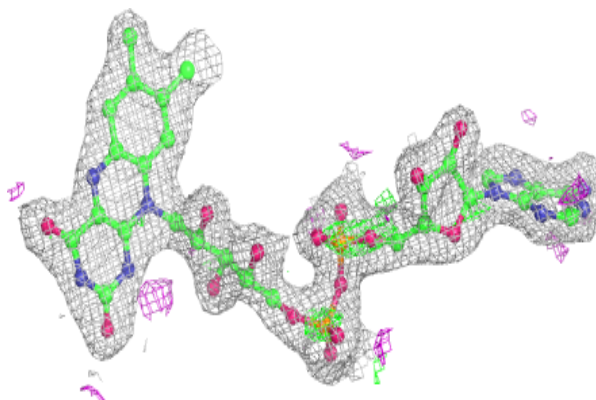mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
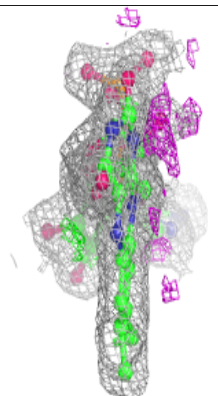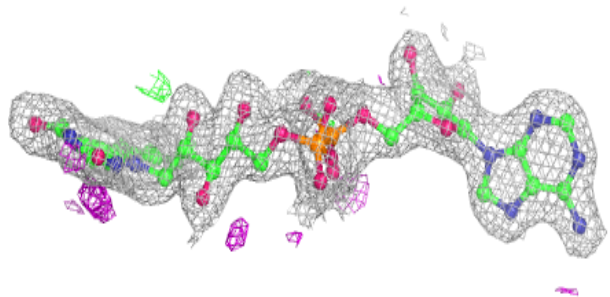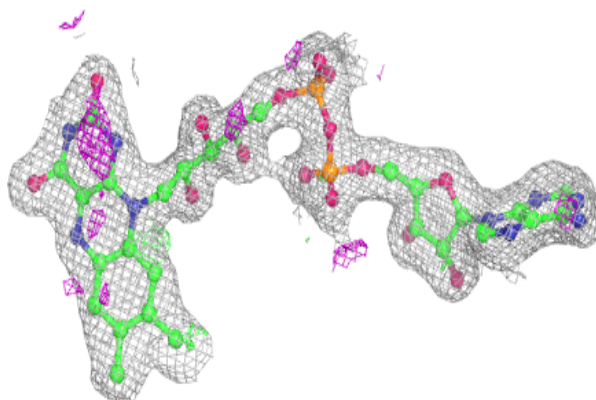
Electron density around FAD C 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
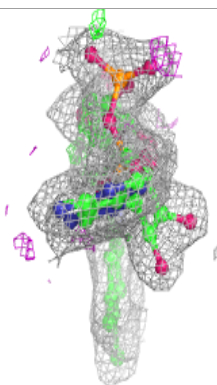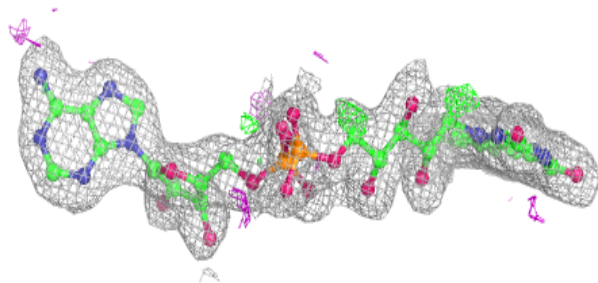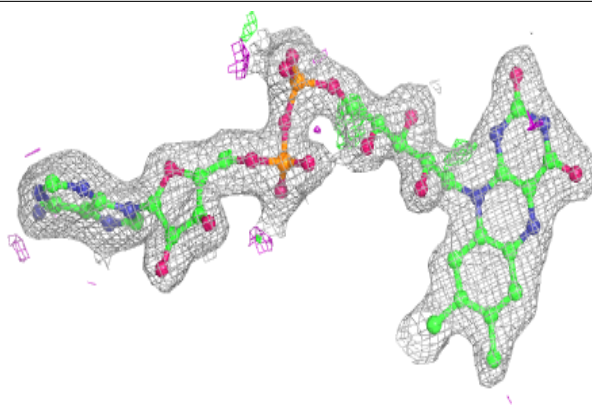
Electron density around FAD H 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
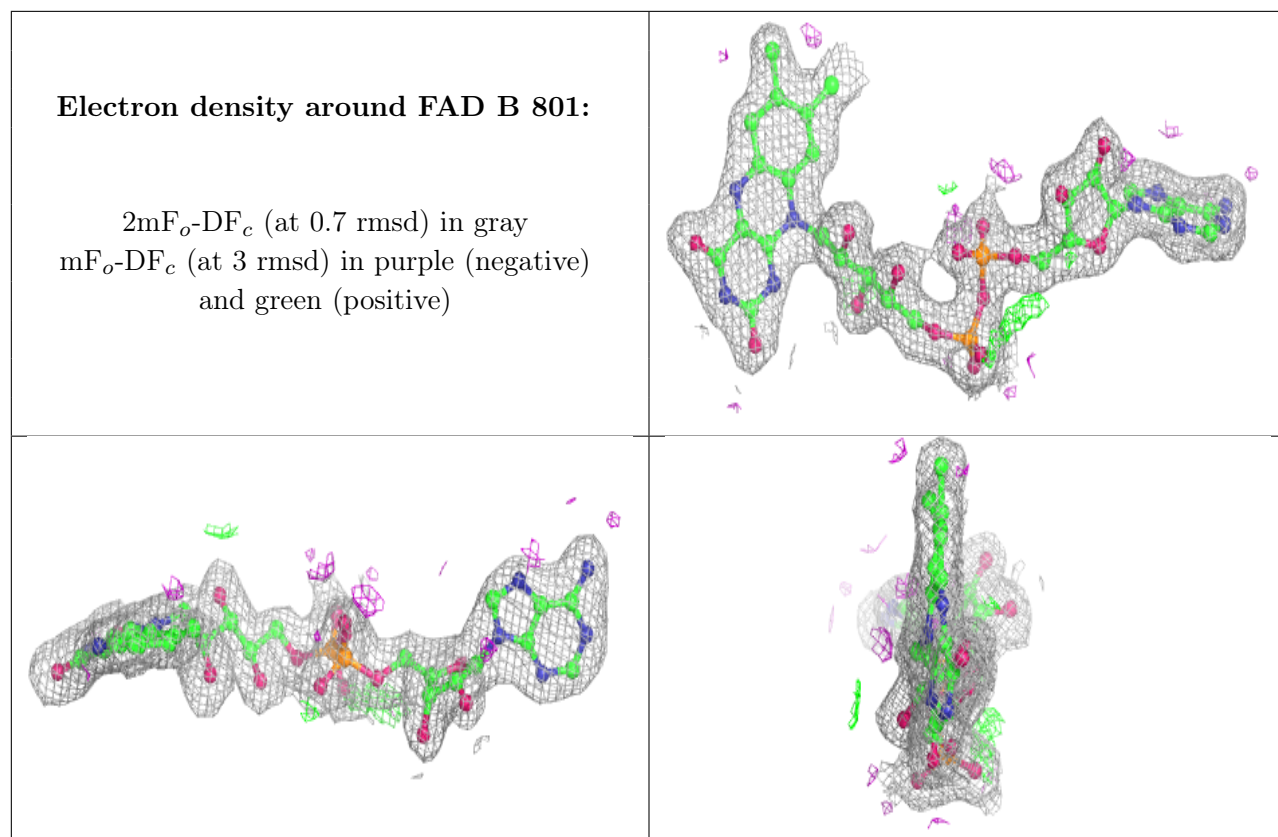mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
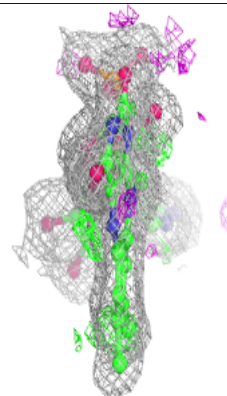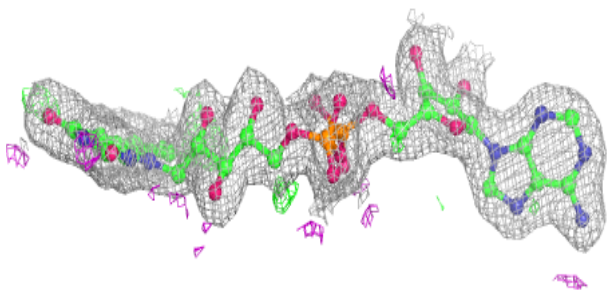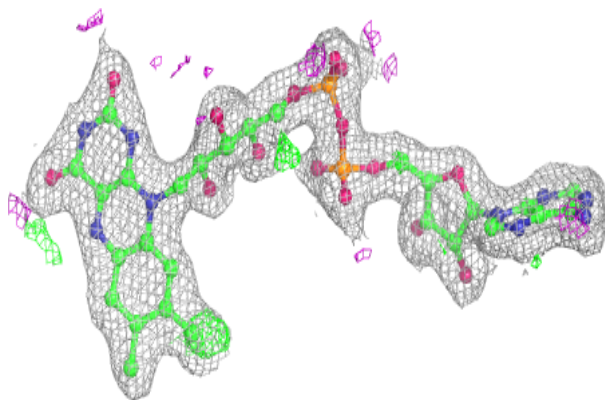
Electron density around FAD A 801:

$2mF_o$-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)

Electron density around FAD B 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 ⓘ

There are no such residues in this entry.