



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:27 AM UTC

PDB ID : 3MPJ / pdb_00003mpj
Title : Structure of the glutaryl-coenzyme A dehydrogenase
Authors : Wischgoll, S.; Warkentin, E.; Boll, M.; Ermler, U.
Deposited on : 2010-04-27
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

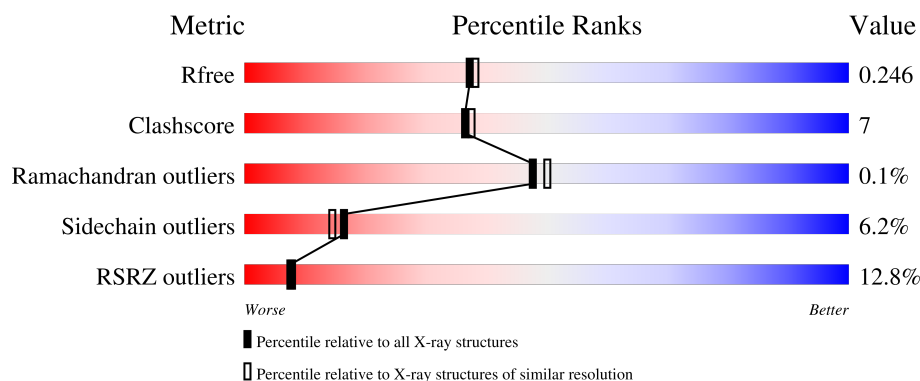
1 Overall quality at a glance

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	397	80% 16% ...
1	B	397	% 81% 15% ...
1	D	397	31% 82% 15% ..
1	E	397	37% 75% 22% ..
1	F	397	% 85% 12% ..

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Mol	Chain	Length	Quality of chain
1	G	397	6% 82% 14%
2	Y	8	50% 12% 62% 12% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19170 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 Glutaryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	2	0
			2992	1891	510	571	20			
1	B	393	Total	C	N	O	S	0	2	0
			3026	1913	520	573	20			
1	D	390	Total	C	N	O	S	0	2	0
			3004	1899	515	570	20			
1	E	391	Total	C	N	O	S	0	1	0
			2999	1896	515	568	20			
1	F	390	Total	C	N	O	S	0	2	0
			3001	1898	514	569	20			
1	G	389	Total	C	N	O	S	0	0	0
			2975	1882	508	565	20			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	390	LYS	-	expression tag	UNP C3UVB0
A	391	GLY	-	expression tag	UNP C3UVB0
A	392	HIS	-	expression tag	UNP C3UVB0
A	393	HIS	-	expression tag	UNP C3UVB0
A	394	HIS	-	expression tag	UNP C3UVB0
A	395	HIS	-	expression tag	UNP C3UVB0
A	396	HIS	-	expression tag	UNP C3UVB0
A	397	HIS	-	expression tag	UNP C3UVB0
B	390	LYS	-	expression tag	UNP C3UVB0
B	391	GLY	-	expression tag	UNP C3UVB0
B	392	HIS	-	expression tag	UNP C3UVB0
B	393	HIS	-	expression tag	UNP C3UVB0
B	394	HIS	-	expression tag	UNP C3UVB0
B	395	HIS	-	expression tag	UNP C3UVB0
B	396	HIS	-	expression tag	UNP C3UVB0
B	397	HIS	-	expression tag	UNP C3UVB0
D	390	LYS	-	expression tag	UNP C3UVB0

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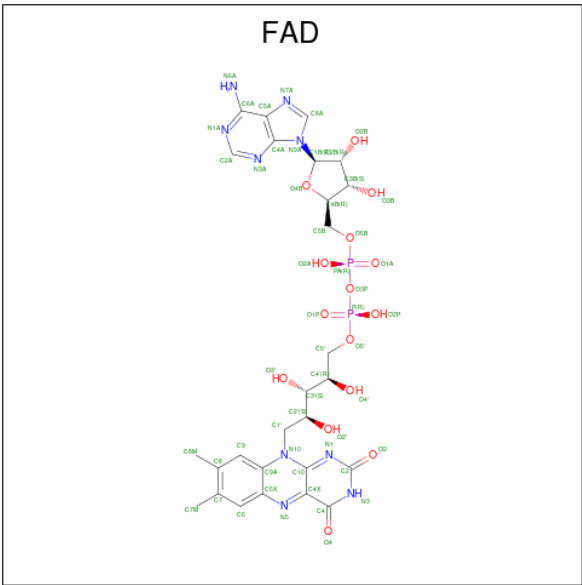
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Chain	Residue	Modelled	Actual	Comment	Reference
D	391	GLY	-	expression tag	UNP C3UVB0
D	392	HIS	-	expression tag	UNP C3UVB0
D	393	HIS	-	expression tag	UNP C3UVB0
D	394	HIS	-	expression tag	UNP C3UVB0
D	395	HIS	-	expression tag	UNP C3UVB0
D	396	HIS	-	expression tag	UNP C3UVB0
D	397	HIS	-	expression tag	UNP C3UVB0
E	390	LYS	-	expression tag	UNP C3UVB0
E	391	GLY	-	expression tag	UNP C3UVB0
E	392	HIS	-	expression tag	UNP C3UVB0
E	393	HIS	-	expression tag	UNP C3UVB0
E	394	HIS	-	expression tag	UNP C3UVB0
E	395	HIS	-	expression tag	UNP C3UVB0
E	396	HIS	-	expression tag	UNP C3UVB0
E	397	HIS	-	expression tag	UNP C3UVB0
F	390	LYS	-	expression tag	UNP C3UVB0
F	391	GLY	-	expression tag	UNP C3UVB0
F	392	HIS	-	expression tag	UNP C3UVB0
F	393	HIS	-	expression tag	UNP C3UVB0
F	394	HIS	-	expression tag	UNP C3UVB0
F	395	HIS	-	expression tag	UNP C3UVB0
F	396	HIS	-	expression tag	UNP C3UVB0
F	397	HIS	-	expression tag	UNP C3UVB0
G	390	LYS	-	expression tag	UNP C3UVB0
G	391	GLY	-	expression tag	UNP C3UVB0
G	392	HIS	-	expression tag	UNP C3UVB0
G	393	HIS	-	expression tag	UNP C3UVB0
G	394	HIS	-	expression tag	UNP C3UVB0
G	395	HIS	-	expression tag	UNP C3UVB0
G	396	HIS	-	expression tag	UNP C3UVB0
G	397	HIS	-	expression tag	UNP C3UVB0

- Molecule 2 is a protein called Octapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Y	8	Total	C	N	O	0	0	0
			72	44	20	8			

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



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		

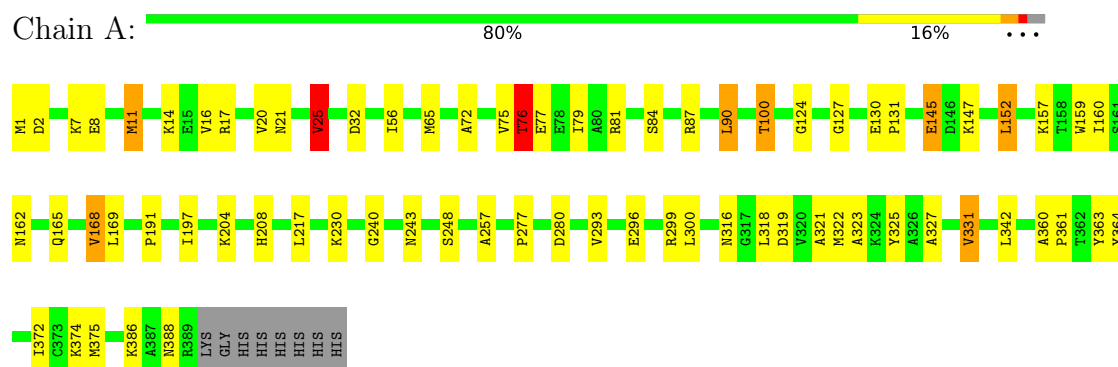
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	175	Total 175	O 175	0	0
5	B	179	Total 179	O 179	0	0
5	D	84	Total 84	O 84	0	0
5	E	78	Total 78	O 78	0	0
5	F	143	Total 143	O 143	0	0
5	G	115	Total 115	O 115	0	0
5	Y	3	Total 3	O 3	0	0

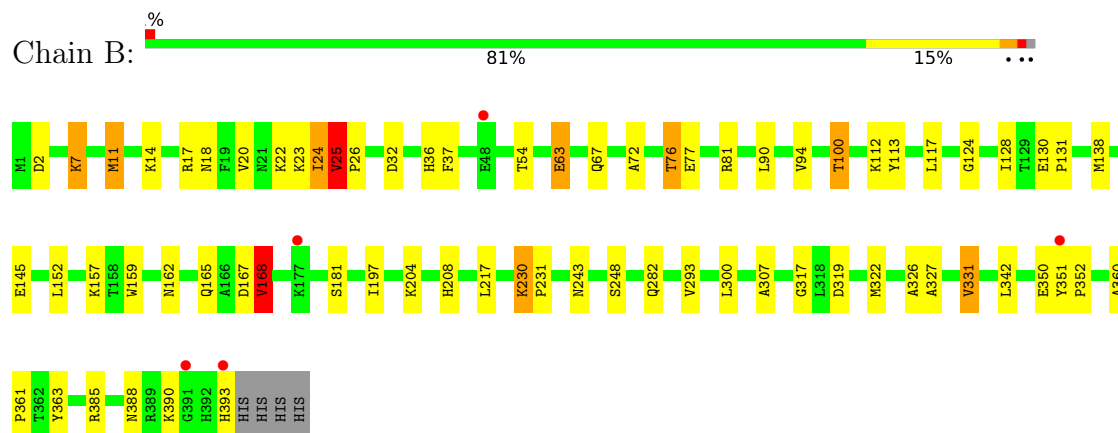
3 Residue-property plots

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.

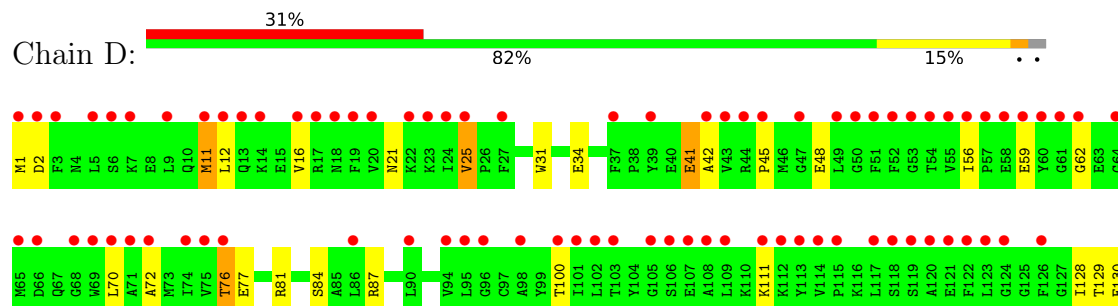
• Molecule 1: Glutaryl-CoA dehydrogenase

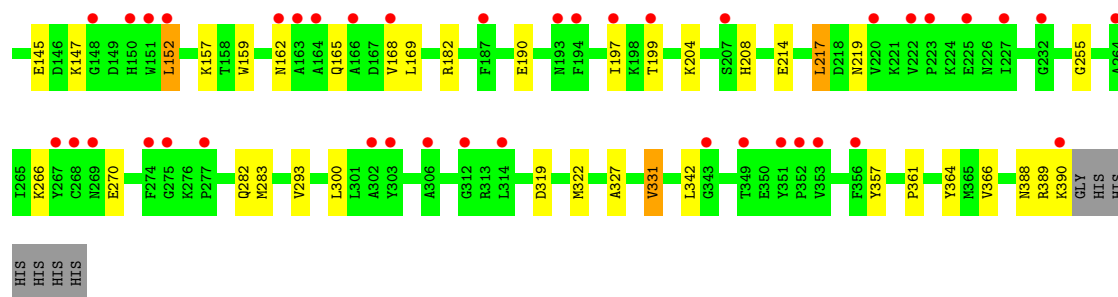


• Molecule 1: Glutaryl-CoA dehydrogenase

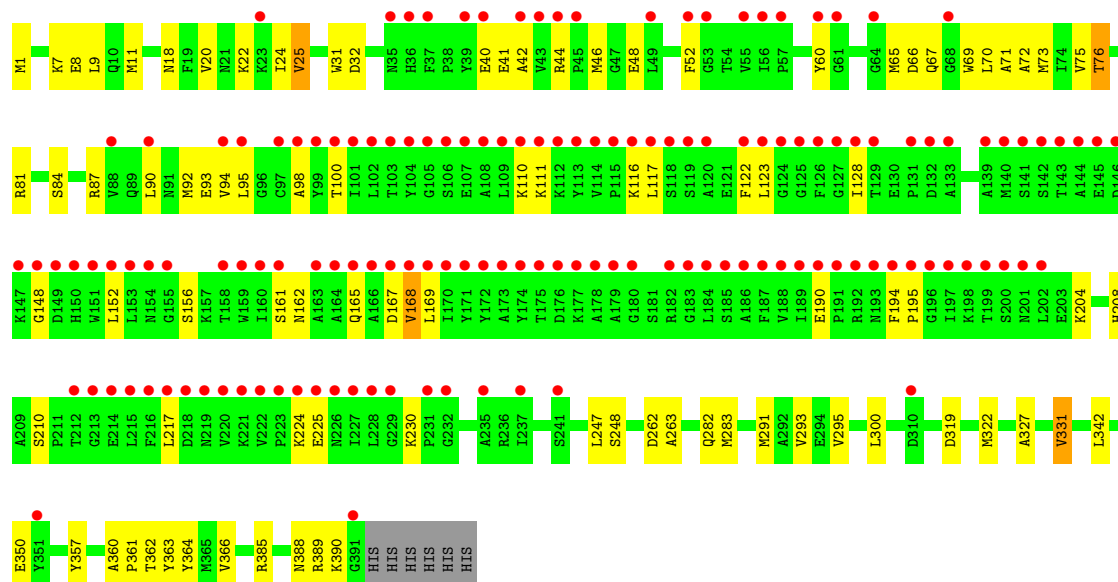
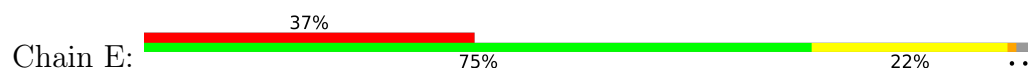


• Molecule 1: Glutaryl-CoA dehydrogenase

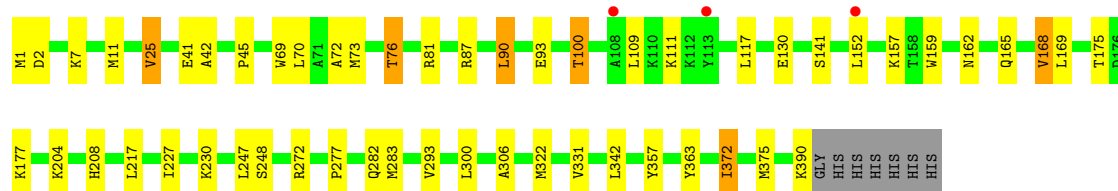
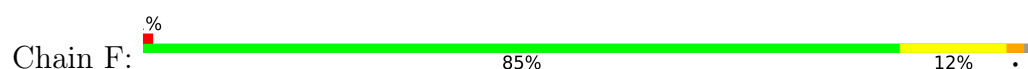




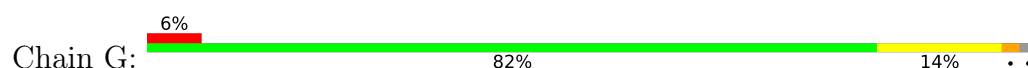
• Molecule 1: Glutaryl-CoA dehydrogenase

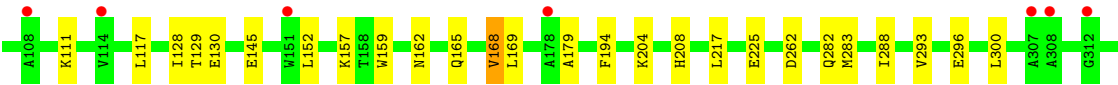


• Molecule 1: Glutaryl-CoA dehydrogenase

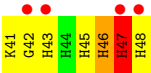
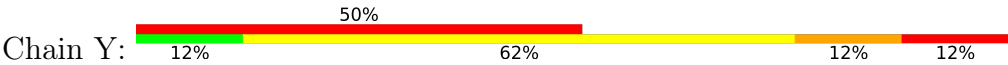


• Molecule 1: Glutaryl-CoA dehydrogenase





● Molecule 2: Octapeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.40Å 250.60Å 62.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.10) 99.7 (30.00-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.181 , 0.225 0.217 , 0.246	Depositor DCC
R_{free} test set	7079 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19170	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 13.59% 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: CL, 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	5/3050 (0.2%)	1.09	4/4117 (0.1%)
1	B	1.10	3/3086 (0.1%)	1.08	5/4163 (0.1%)
1	D	0.86	1/3062 (0.0%)	0.99	1/4131 (0.0%)
1	E	0.85	1/3057 (0.0%)	1.04	8/4124 (0.2%)
1	F	1.00	2/3062 (0.1%)	1.03	1/4131 (0.0%)
1	G	0.95	3/3033 (0.1%)	1.00	1/4094 (0.0%)
2	Y	0.96	0/76	1.23	1/98 (1.0%)
All	All	0.98	15/18426 (0.1%)	1.04	21/24858 (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
2	Y	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	25	VAL	CA-CB	12.02	1.62	1.53
1	B	25	VAL	CA-CB	9.97	1.60	1.53
1	A	160	ILE	CA-CB	6.51	1.61	1.53
1	G	76	THR	CA-CB	6.44	1.63	1.53
1	F	227	ILE	CA-CB	6.19	1.61	1.54
1	A	257	ALA	CA-CB	6.14	1.62	1.53
1	F	372	ILE	CA-CB	6.06	1.62	1.54
1	A	56	ILE	CA-CB	5.65	1.61	1.54
1	E	263	ALA	CA-CB	-5.65	1.44	1.53
1	A	25	VAL	CA-CB	5.64	1.61	1.54
1	G	288	ILE	CA-CB	5.63	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	VAL	C-O	5.51	1.29	1.24
1	B	307	ALA	CA-CB	5.32	1.61	1.53
1	A	76	THR	CA-CB	5.26	1.61	1.53
1	G	38	PRO	N-CA	5.06	1.51	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	VAL	N-CA-CB	11.84	117.96	110.50
1	D	25	VAL	N-CA-CB	9.65	116.58	110.50
1	E	389	ARG	N-CA-C	7.87	123.42	112.72
2	Y	47	HIS	N-CA-C	-7.10	98.52	109.24
1	E	190	GLU	CA-C-N	6.10	125.58	119.24
1	E	190	GLU	C-N-CA	6.10	125.58	119.24
1	G	129	THR	N-CA-C	6.02	118.96	110.23
1	B	94	VAL	N-CA-C	6.00	117.12	111.48
1	E	390	LYS	N-CA-C	5.98	119.63	112.93
1	A	323	ALA	N-CA-C	-5.92	104.83	111.28
1	A	76	THR	N-CA-CB	5.89	118.87	110.16
1	E	230	LYS	N-CA-C	-5.62	103.66	110.13
1	A	25	VAL	N-CA-CB	5.58	119.03	111.21
1	B	24	ILE	CA-C-N	-5.44	116.81	120.24
1	B	24	ILE	C-N-CA	-5.44	116.81	120.24
1	E	25	VAL	CA-C-N	-5.42	114.09	119.56
1	E	25	VAL	C-N-CA	-5.42	114.09	119.56
1	B	326	ALA	N-CA-C	-5.24	105.65	111.36
1	E	363	TYR	N-CA-C	5.18	118.85	112.54
1	A	321	ALA	N-CA-C	-5.02	105.89	111.36
1	F	25	VAL	N-CA-CB	5.02	118.24	111.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	46	HIS	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	2992	0	2945	51	0
1	B	3026	0	2984	50	0
1	D	3004	0	2967	41	0
1	E	2999	0	2965	54	0
1	F	3001	0	2968	35	1
1	G	2975	0	2937	46	0
2	Y	72	0	55	8	1
3	A	53	0	31	4	0
3	B	53	0	31	4	0
3	D	53	0	31	5	0
3	E	53	0	31	4	0
3	F	53	0	31	5	0
3	G	53	0	31	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	175	0	0	6	0
5	B	179	0	0	6	0
5	D	84	0	0	1	0
5	E	78	0	0	2	0
5	F	143	0	0	4	1
5	G	115	0	0	2	1
5	Y	3	0	0	0	0
All	All	19170	0	18007	263	2

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 7.

All (263) 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:G:72:ALA:O	1:G:76:THR:HG22	1.65	0.95
2:Y:42:GLY:C	2:Y:43:HIS:CA	2.48	0.86
1:F:331:VAL:HG21	1:F:363:TYR:HB2	1.59	0.84
5:B:7089:HOH:O	2:Y:47:HIS:HB3	1.77	0.84
1:E:72:ALA:O	1:E:76:THR:HG22	1.78	0.83
1:B:36:HIS:HD2	2:Y:48:HIS:HA	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:46:HIS:HB2	2:Y:48:HIS:HD2	1.44	0.83
1:B:11:MET:HE2	1:B:14:LYS:HD2	1.62	0.81
1:B:77:GLU:OE1	5:B:7219:HOH:O	1.98	0.81
1:D:72:ALA:O	1:D:76:THR:HG22	1.79	0.81
1:D:70:LEU:HD21	1:G:1:MET:HG2	1.63	0.80
1:B:76:THR:HG22	1:B:90:LEU:HD23	1.61	0.80
1:F:100:THR:HG21	5:F:7538:HOH:O	1.80	0.79
1:G:327:ALA:O	1:G:331:VAL:HG12	1.84	0.78
2:Y:46:HIS:HB2	2:Y:48:HIS:CD2	2.18	0.77
1:G:72:ALA:O	1:G:76:THR:CG2	2.33	0.77
1:E:72:ALA:O	1:E:76:THR:CG2	2.35	0.75
1:B:327:ALA:O	1:B:331:VAL:HG13	1.86	0.74
1:A:327:ALA:O	1:A:331:VAL:HG13	1.87	0.73
1:A:77:GLU:OE1	5:A:7266:HOH:O	2.09	0.70
1:D:81[B]:ARG:O	1:D:81[B]:ARG:HG2	1.93	0.68
3:E:400:FAD:H2'	3:E:400:FAD:H9	1.76	0.67
3:D:400:FAD:H2'	3:D:400:FAD:C9	2.25	0.67
3:F:400:FAD:H2'	3:F:400:FAD:H9	1.76	0.67
1:A:81:ARG:HD2	5:A:7957:HOH:O	1.93	0.67
3:F:400:FAD:H2'	3:F:400:FAD:C9	2.24	0.67
1:G:17:ARG:HH12	1:G:81:ARG:HH21	1.40	0.67
3:G:400:FAD:H2'	3:G:400:FAD:C9	2.24	0.66
3:E:400:FAD:H2'	3:E:400:FAD:C9	2.25	0.66
1:A:76:THR:HG22	1:A:90:LEU:HD23	1.77	0.66
1:A:322:MET:CE	1:B:293:VAL:HA	2.24	0.66
1:A:322:MET:HE3	1:B:293:VAL:HA	1.77	0.65
1:F:272:ARG:NH1	1:F:277:PRO:HD3	2.13	0.64
1:G:17:ARG:HH12	1:G:81:ARG:NH2	1.95	0.64
1:F:72:ALA:O	1:F:76:THR:HG22	1.97	0.64
1:E:282:GLN:HE21	1:G:283:MET:H	1.46	0.64
1:E:283:MET:H	1:G:282:GLN:HE21	1.46	0.64
1:A:331:VAL:HG21	1:A:363:TYR:HB2	1.80	0.64
1:D:282:GLN:HE21	1:F:283:MET:H	1.45	0.64
1:A:293:VAL:HA	1:B:322:MET:HE3	1.80	0.63
1:E:162:ASN:HA	1:E:165:GLN:HE21	1.62	0.63
1:G:5:LEU:O	1:G:10:GLN:NE2	2.31	0.63
1:B:204:LYS:O	1:B:208:HIS:HE1	1.80	0.63
1:E:8:GLU:HG2	1:E:65:MET:HE3	1.81	0.63
1:F:81:ARG:HD2	5:F:7589:HOH:O	1.98	0.63
3:G:400:FAD:H2'	3:G:400:FAD:H9	1.80	0.63
1:D:283:MET:H	1:F:282:GLN:HE21	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:ARG:HD2	5:E:7641:HOH:O	1.99	0.62
1:E:331:VAL:HG23	1:E:360:ALA:HB1	1.80	0.62
1:E:327:ALA:O	1:E:331:VAL:HG13	2.00	0.61
1:B:36:HIS:CD2	2:Y:48:HIS:HA	2.32	0.61
1:E:20:VAL:HG22	1:E:24:ILE:HD12	1.83	0.61
1:D:322:MET:HE1	1:G:296:GLU:HB3	1.82	0.61
1:D:322:MET:HE3	1:G:293:VAL:HA	1.82	0.61
1:E:18:ASN:HD21	1:E:22:LYS:NZ	2.00	0.60
3:B:400:FAD:H2'	3:B:400:FAD:C9	2.31	0.60
1:E:293:VAL:HA	1:F:322:MET:HE3	1.84	0.60
1:G:204:LYS:O	1:G:208:HIS:HE1	1.84	0.59
1:G:35:ASN:HD22	1:G:208:HIS:HB3	1.66	0.59
1:D:21:ASN:ND2	1:D:81[B]:ARG:HH22	2.00	0.59
1:D:130:GLU:HG2	1:D:157:LYS:HD3	1.85	0.59
1:E:322:MET:HE3	1:F:293:VAL:HA	1.83	0.59
1:G:35:ASN:ND2	1:G:208:HIS:HB3	2.17	0.59
1:A:159:TRP:O	3:A:400:FAD:C4X	2.50	0.59
1:G:21:ASN:HA	1:G:25:VAL:HG13	1.85	0.59
1:G:11:MET:HE2	1:G:14:LYS:HD2	1.84	0.59
1:G:162:ASN:HA	1:G:165:GLN:HE21	1.68	0.58
1:E:293:VAL:HA	1:F:322:MET:CE	2.33	0.58
1:F:100:THR:HG22	5:F:7633:HOH:O	2.02	0.58
1:A:21:ASN:HA	1:A:25:VAL:HG13	1.86	0.58
1:E:1:MET:HG2	1:F:70:LEU:HD21	1.85	0.58
1:D:152:LEU:HD21	1:D:219:ASN:HA	1.86	0.57
1:E:282:GLN:HB2	1:G:282:GLN:HB2	1.86	0.57
1:A:17:ARG:HH12	1:A:81:ARG:NH2	2.02	0.57
1:F:72:ALA:O	1:F:76:THR:CG2	2.52	0.57
1:D:1:MET:HG2	1:G:70:LEU:HD21	1.85	0.57
1:E:87:ARG:HD2	1:E:87:ARG:C	2.30	0.57
1:E:117:LEU:HD21	1:E:168:VAL:CG1	2.34	0.57
1:D:199:THR:HA	1:D:214:GLU:O	2.05	0.56
1:B:319:ASP:H	1:B:388:ASN:HD21	1.54	0.56
1:G:81:ARG:NH1	1:G:262:ASP:OD2	2.38	0.56
1:B:72:ALA:O	1:B:76:THR:CG2	2.53	0.56
1:D:12:LEU:O	1:D:16:VAL:HG23	2.06	0.56
1:A:319:ASP:H	1:A:388:ASN:HD21	1.53	0.56
1:E:44:ARG:NH1	1:E:48:GLU:HG3	2.21	0.56
1:D:319:ASP:H	1:D:388:ASN:HD21	1.53	0.56
1:F:357:TYR:CE2	1:G:357:TYR:CE2	2.94	0.56
1:A:100:THR:HG21	5:A:7065:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ALA:O	1:E:46:MET:HG3	2.05	0.56
1:D:31:TRP:CZ2	1:D:41:GLU:HG3	2.41	0.55
1:A:72:ALA:O	1:A:76:THR:CG2	2.55	0.55
3:E:400:FAD:H2A	1:F:282:GLN:HE22	1.72	0.55
1:D:147:LYS:HE3	1:D:152:LEU:HD12	1.89	0.55
1:B:124:GLY:HA2	1:B:168:VAL:O	2.06	0.55
1:E:319:ASP:H	1:E:388:ASN:HD21	1.55	0.54
1:B:130:GLU:HG2	1:B:157:LYS:HD3	1.90	0.54
1:A:145[B]:GLU:OE2	1:A:147:LYS:NZ	2.27	0.54
1:A:240:GLY:HA3	5:A:7283:HOH:O	2.07	0.54
1:D:84:SER:O	1:D:87:ARG:HG3	2.07	0.54
1:A:318:LEU:H	1:A:388:ASN:ND2	2.06	0.54
1:E:81:ARG:NH1	1:E:262:ASP:OD2	2.41	0.54
1:G:130:GLU:HG2	1:G:157:LYS:HD3	1.90	0.54
1:D:327:ALA:O	1:D:331:VAL:HG13	2.07	0.53
1:G:87:ARG:HD2	1:G:87:ARG:C	2.33	0.53
1:A:72:ALA:O	1:A:76:THR:HG22	2.09	0.53
1:G:17:ARG:NH1	1:G:81:ARG:NH2	2.57	0.53
3:A:400:FAD:C9	3:A:400:FAD:H2'	2.39	0.53
1:B:72:ALA:O	1:B:76:THR:HG22	2.08	0.53
1:E:84:SER:O	1:E:87:ARG:HG3	2.09	0.52
1:A:16:VAL:O	1:A:20:VAL:HG23	2.10	0.52
1:G:318:LEU:O	1:G:322:MET:HG3	2.10	0.52
1:B:162:ASN:HA	1:B:165:GLN:HE21	1.75	0.52
1:D:389:ARG:O	1:D:390:LYS:C	2.51	0.52
1:B:100:THR:HG21	5:B:7078:HOH:O	2.09	0.52
1:A:100:THR:HG22	5:A:7075:HOH:O	2.09	0.51
1:A:296:GLU:HB3	1:B:322:MET:HE1	1.92	0.51
1:E:70:LEU:HD21	1:F:1:MET:HG2	1.91	0.51
3:D:400:FAD:H2'	3:D:400:FAD:H9	1.92	0.51
1:D:282:GLN:HB2	1:F:282:GLN:HB2	1.93	0.51
1:B:76:THR:CG2	1:B:90:LEU:HD23	2.37	0.51
1:A:277:PRO:HD2	1:A:280:ASP:OD2	2.11	0.51
1:F:162:ASN:HA	1:F:165:GLN:HE21	1.76	0.50
1:G:100:THR:HG21	5:G:7411:HOH:O	2.10	0.50
3:A:400:FAD:H2A	1:B:282:GLN:HE22	1.76	0.50
1:D:56:ILE:HB	1:D:62:GLY:HA3	1.94	0.50
1:E:116:LYS:HD2	1:E:122:PHE:CZ	2.47	0.50
1:G:117:LEU:HD21	1:G:168:VAL:HG13	1.92	0.50
1:B:167:ASP:OD2	2:Y:45:HIS:HE1	1.95	0.50
1:D:162:ASN:HA	1:D:165:GLN:HE21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:MET:H	1:G:282:GLN:NE2	2.09	0.50
1:D:21:ASN:HD21	1:D:81[B]:ARG:HH22	1.60	0.49
1:B:243:ASN:HD21	1:B:317:GLY:HA2	1.77	0.49
1:F:73:MET:HG3	1:F:306:ALA:HB2	1.94	0.49
1:B:20:VAL:HG22	1:B:24:ILE:HD12	1.93	0.49
1:A:243:ASN:HB3	5:A:7130:HOH:O	2.13	0.49
1:D:282:GLN:NE2	1:F:283:MET:H	2.10	0.49
1:A:372:ILE:HA	1:A:375:MET:HE3	1.95	0.49
1:B:385:ARG:HG3	1:B:385:ARG:HH11	1.78	0.49
1:E:60:TYR:CZ	1:E:110:LYS:HD2	2.48	0.49
1:E:204:LYS:O	1:E:208:HIS:HE1	1.96	0.48
1:B:112:LYS:HE2	1:B:113:TYR:OH	2.13	0.48
1:A:11:MET:HE2	1:A:14:LYS:HD2	1.95	0.48
1:E:116:LYS:HB2	1:E:122:PHE:CD2	2.49	0.48
1:G:331:VAL:HG11	1:G:363:TYR:CB	2.44	0.48
1:E:32:ASP:OD1	1:E:208:HIS:HD2	1.97	0.48
1:E:94:VAL:HA	1:E:98:ALA:HB3	1.94	0.48
1:G:56:ILE:HB	1:G:62:GLY:HA3	1.96	0.48
1:F:272:ARG:HH12	1:F:277:PRO:HD3	1.79	0.48
1:B:331:VAL:HG21	1:B:363:TYR:HB2	1.95	0.48
1:E:71:ALA:O	1:E:75:VAL:HG23	2.14	0.48
1:E:73:MET:SD	1:E:247:LEU:HG	2.53	0.48
1:F:42:ALA:C	1:F:45:PRO:HD2	2.39	0.47
1:A:32:ASP:OD1	1:A:208:HIS:HD2	1.98	0.47
1:A:1:MET:HE2	1:A:1:MET:HB2	1.80	0.47
1:E:92:MET:SD	1:E:161:SER:HB2	2.55	0.47
1:D:357:TYR:CE2	1:E:357:TYR:CE2	3.03	0.47
1:E:282:GLN:HE22	3:F:400:FAD:H2A	1.79	0.47
1:A:127:GLY:O	1:A:157:LYS:HE3	2.15	0.47
1:E:282:GLN:NE2	1:G:283:MET:H	2.13	0.47
1:E:128:ILE:HB	3:E:400:FAD:O2	2.16	0.46
1:B:100:THR:HG22	5:B:7158:HOH:O	2.15	0.46
1:D:152:LEU:CD2	1:D:219:ASN:HA	2.46	0.46
1:B:243:ASN:ND2	1:B:317:GLY:HA2	2.30	0.46
1:D:283:MET:H	1:F:282:GLN:NE2	2.12	0.46
1:D:293:VAL:HA	1:G:322:MET:HE2	1.98	0.46
3:B:400:FAD:H2'	3:B:400:FAD:H9	1.97	0.46
1:A:204:LYS:O	1:A:208:HIS:HE1	1.98	0.46
1:D:204:LYS:O	1:D:208:HIS:HE1	1.98	0.46
1:E:282:GLN:HB3	1:G:283:MET:HG3	1.98	0.46
1:A:130:GLU:HG2	1:A:157:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:GLU:HB3	5:D:7587:HOH:O	2.15	0.46
1:D:197:ILE:HG12	1:D:217:LEU:HD22	1.97	0.46
1:E:18:ASN:HD21	1:E:22:LYS:HZ3	1.62	0.46
1:B:17:ARG:HH12	1:B:81:ARG:NH2	2.14	0.46
1:D:77:GLU:HG2	1:D:255:GLY:HA2	1.97	0.46
1:D:159:TRP:O	3:D:400:FAD:C4X	2.64	0.46
1:E:81:ARG:NH2	5:E:7557:HOH:O	2.46	0.46
3:F:400:FAD:H9	3:F:400:FAD:C2'	2.44	0.46
1:F:76:THR:HG21	1:F:248:SER:OG	2.16	0.45
1:A:8:GLU:HG2	1:A:65:MET:CE	2.46	0.45
1:D:42:ALA:C	1:D:45:PRO:HD2	2.41	0.45
1:B:360:ALA:N	1:B:361:PRO:CD	2.80	0.45
1:F:109:LEU:HD12	5:F:7583:HOH:O	2.17	0.45
1:G:194:PHE:N	1:G:194:PHE:CD1	2.83	0.45
1:B:159:TRP:O	3:B:400:FAD:C4X	2.64	0.45
1:D:361:PRO:HA	1:D:364:TYR:CZ	2.52	0.45
1:B:18:ASN:HD21	1:B:22:LYS:NZ	2.14	0.45
1:D:266:LYS:HE2	1:D:270:GLU:OE1	2.16	0.45
1:F:130:GLU:HG2	1:F:157:LYS:HD3	1.98	0.45
1:E:52:PHE:O	1:E:94:VAL:HG21	2.16	0.45
1:F:73:MET:SD	1:F:247:LEU:HG	2.56	0.45
1:F:76:THR:HG22	1:F:90:LEU:HD23	1.99	0.45
1:B:197:ILE:HG12	1:B:217:LEU:HD22	2.00	0.44
1:D:128:ILE:HB	3:D:400:FAD:O2	2.17	0.44
1:A:360:ALA:N	1:A:361:PRO:CD	2.80	0.44
1:A:159:TRP:O	3:A:400:FAD:C10	2.66	0.44
1:D:129:THR:OG1	3:D:400:FAD:H1'1	2.17	0.44
1:A:17:ARG:HH12	1:A:81:ARG:CZ	2.30	0.44
1:E:69:TRP:O	1:E:73:MET:HG2	2.17	0.44
1:F:204:LYS:O	1:F:208:HIS:HE1	2.01	0.44
1:B:76:THR:HG21	1:B:248:SER:OG	2.18	0.43
1:E:291:MET:O	1:E:295:VAL:HG23	2.18	0.43
1:B:138:MET:HE2	1:B:181:SER:HA	2.00	0.43
1:B:351:TYR:HB3	1:B:352:PRO:HD2	2.01	0.43
1:D:11:MET:HE3	1:D:11:MET:HA	1.99	0.43
1:F:141:SER:O	1:F:177:LYS:NZ	2.40	0.43
1:E:123:LEU:HD13	1:E:165:GLN:HB3	2.00	0.43
1:A:145[A]:GLU:HG2	1:A:152:LEU:O	2.18	0.43
1:B:7:LYS:HD2	1:B:7:LYS:HA	1.74	0.43
1:E:194:PHE:HA	1:E:195:PRO:HD3	1.88	0.43
1:E:31:TRP:CZ2	1:E:41:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:LEU:HD12	1:E:248:SER:HB2	2.00	0.43
1:G:159:TRP:O	3:G:400:FAD:C4X	2.67	0.43
1:A:76:THR:HG21	1:A:248:SER:OG	2.19	0.43
1:B:72:ALA:O	1:B:76:THR:HG23	2.17	0.43
1:E:361:PRO:HA	1:E:364:TYR:CZ	2.53	0.43
1:F:117:LEU:HD21	1:F:168:VAL:HG13	2.00	0.43
1:A:316:ASN:C	1:A:388:ASN:HD22	2.27	0.43
1:A:84:SER:O	1:A:87:ARG:HG3	2.19	0.42
1:G:204:LYS:O	1:G:208:HIS:CE1	2.70	0.42
1:A:72:ALA:O	1:A:76:THR:HG23	2.19	0.42
1:B:54:THR:HA	1:B:63:GLU:HB2	2.01	0.42
1:G:99:TYR:O	1:G:102:LEU:HB3	2.19	0.42
1:G:81:ARG:HD2	5:G:7596:HOH:O	2.18	0.42
1:B:67:GLN:NE2	5:B:7247:HOH:O	2.20	0.42
1:E:9:LEU:HD11	1:E:67:GLN:HE21	1.85	0.42
1:A:130:GLU:O	1:A:131:PRO:C	2.61	0.42
1:E:116:LYS:HB2	1:E:122:PHE:CE2	2.55	0.42
1:A:75:VAL:O	1:A:79:ILE:HG13	2.20	0.42
1:A:325:TYR:CE1	1:A:374:LYS:HE3	2.55	0.42
1:G:331:VAL:HG11	1:G:363:TYR:HB2	2.02	0.42
1:A:191:PRO:HA	1:A:197:ILE:HD13	2.02	0.42
1:E:122:PHE:HA	1:E:167:ASP:OD2	2.20	0.42
1:B:32:ASP:OD1	1:B:208:HIS:HD2	2.03	0.41
1:F:372:ILE:HA	1:F:375:MET:HE3	2.02	0.41
1:B:128:ILE:HB	3:B:400:FAD:O2	2.21	0.41
1:G:319:ASP:H	1:G:388:ASN:HD21	1.67	0.41
1:B:25:VAL:N	1:B:26:PRO:CD	2.83	0.41
1:D:31:TRP:HZ2	1:D:41:GLU:HG3	1.82	0.41
1:E:73:MET:HE2	1:E:73:MET:HA	2.02	0.41
1:F:87:ARG:C	1:F:87:ARG:HD2	2.44	0.41
1:A:322:MET:HE3	1:B:293:VAL:HG22	2.03	0.41
1:G:11:MET:HA	1:G:11:MET:HE3	2.01	0.41
1:B:230:LYS:O	1:B:231:PRO:C	2.61	0.41
1:A:124:GLY:HA2	1:A:168:VAL:O	2.21	0.41
1:G:225:GLU:H	1:G:225:GLU:CD	2.28	0.41
1:E:362:THR:O	1:E:366:VAL:HG22	2.21	0.41
1:G:128:ILE:HB	3:G:400:FAD:O2	2.20	0.41
1:A:7:LYS:HD2	1:A:7:LYS:HA	1.57	0.41
1:F:69:TRP:O	1:F:73:MET:HG2	2.20	0.41
1:G:19:PHE:CE2	1:G:46:MET:CG	3.03	0.41
1:G:31:TRP:CE3	1:G:38:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145[B]:GLU:CD	1:A:147:LYS:HZ3	2.20	0.41
1:A:299:ARG:HH11	1:A:299:ARG:HD2	1.70	0.41
1:F:159:TRP:O	3:F:400:FAD:C4X	2.69	0.41
1:B:117:LEU:HD21	1:B:168:VAL:HG13	2.03	0.40
1:B:37:PHE:HB3	2:Y:47:HIS:H	1.87	0.40
1:B:23:LYS:HE2	1:B:23:LYS:HB3	1.95	0.40
1:A:162:ASN:HA	1:A:165:GLN:HE21	1.87	0.40
1:A:296:GLU:CB	1:B:322:MET:HE1	2.50	0.40
1:B:81:ARG:NH2	5:B:8022:HOH:O	2.30	0.40
1:D:70:LEU:CD2	1:G:1:MET:HG2	2.43	0.40
1:A:361:PRO:HA	1:A:364:TYR:CZ	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:LYS:O	2:Y:41:LYS:CG[4_455]	1.78	0.42
5:F:7936:HOH:O	5:G:8014:HOH:O[1_556]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	389/397 (98%)	376 (97%)	13 (3%)	0	100	100
1	B	393/397 (99%)	380 (97%)	13 (3%)	0	100	100
1	D	390/397 (98%)	379 (97%)	11 (3%)	0	100	100
1	E	390/397 (98%)	368 (94%)	21 (5%)	1 (0%)	36	36
1	F	390/397 (98%)	378 (97%)	12 (3%)	0	100	100
1	G	387/397 (98%)	375 (97%)	11 (3%)	1 (0%)	36	36
2	Y	4/8 (50%)	2 (50%)	2 (50%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2343/2390 (98%)	2258 (96%)	83 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	179	ALA
1	E	148	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	304/309 (98%)	287 (94%)	17 (6%)	19	18
1	B	307/309 (99%)	288 (94%)	19 (6%)	16	14
1	D	305/309 (99%)	284 (93%)	21 (7%)	14	12
1	E	304/309 (98%)	280 (92%)	24 (8%)	11	9
1	F	305/309 (99%)	287 (94%)	18 (6%)	18	16
1	G	302/309 (98%)	285 (94%)	17 (6%)	19	18
2	Y	6/7 (86%)	5 (83%)	1 (17%)	2	1
All	All	1833/1861 (98%)	1716 (94%)	117 (6%)	16	14

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	11	MET
1	A	25	VAL
1	A	76	THR
1	A	90	LEU
1	A	100	THR
1	A	145[A]	GLU
1	A	145[B]	GLU
1	A	152	LEU

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Mol	Chain	Res	Type
1	A	168	VAL
1	A	169	LEU
1	A	217	LEU
1	A	230	LYS
1	A	300	LEU
1	A	331	VAL
1	A	342	LEU
1	A	386	LYS
1	B	2	ASP
1	B	7	LYS
1	B	11	MET
1	B	25	VAL
1	B	63	GLU
1	B	76	THR
1	B	100	THR
1	B	131	PRO
1	B	145[A]	GLU
1	B	145[B]	GLU
1	B	152	LEU
1	B	168	VAL
1	B	230	LYS
1	B	300	LEU
1	B	331	VAL
1	B	342	LEU
1	B	350	GLU
1	B	390	LYS
1	B	393	HIS
1	D	2	ASP
1	D	11	MET
1	D	25	VAL
1	D	34	GLU
1	D	41	GLU
1	D	48	GLU
1	D	59	GLU
1	D	76	THR
1	D	100	THR
1	D	111	LYS
1	D	145[A]	GLU
1	D	145[B]	GLU
1	D	152	LEU
1	D	168	VAL
1	D	169	LEU

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Mol	Chain	Res	Type
1	D	182	ARG
1	D	217	LEU
1	D	300	LEU
1	D	331	VAL
1	D	342	LEU
1	D	366	VAL
1	E	7	LYS
1	E	11	MET
1	E	25	VAL
1	E	40	GLU
1	E	66	ASP
1	E	76	THR
1	E	90	LEU
1	E	93	GLU
1	E	100	THR
1	E	111	LYS
1	E	152	LEU
1	E	156	SER
1	E	168	VAL
1	E	169	LEU
1	E	210	SER
1	E	217	LEU
1	E	224	LYS
1	E	225	GLU
1	E	300	LEU
1	E	331	VAL
1	E	342	LEU
1	E	350	GLU
1	E	385[A]	ARG
1	E	385[B]	ARG
1	F	2	ASP
1	F	7	LYS
1	F	11	MET
1	F	25	VAL
1	F	41	GLU
1	F	76	THR
1	F	90	LEU
1	F	93	GLU
1	F	100	THR
1	F	111	LYS
1	F	152	LEU
1	F	168	VAL

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Mol	Chain	Res	Type
1	F	169	LEU
1	F	175	THR
1	F	217	LEU
1	F	230	LYS
1	F	300	LEU
1	F	342	LEU
1	G	2	ASP
1	G	7	LYS
1	G	11	MET
1	G	25	VAL
1	G	41	GLU
1	G	76	THR
1	G	100	THR
1	G	111	LYS
1	G	145	GLU
1	G	152	LEU
1	G	168	VAL
1	G	169	LEU
1	G	217	LEU
1	G	300	LEU
1	G	331	VAL
1	G	342	LEU
1	G	385	ARG
2	Y	47	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	21	ASN
1	A	33	ASN
1	A	165	GLN
1	A	208	HIS
1	A	243	ASN
1	A	269	ASN
1	A	388	ASN
1	B	18	ASN
1	B	21	ASN
1	B	33	ASN
1	B	36	HIS
1	B	165	GLN
1	B	208	HIS

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Mol	Chain	Res	Type
1	B	226	ASN
1	B	269	ASN
1	B	282	GLN
1	B	388	ASN
1	D	21	ASN
1	D	35	ASN
1	D	165	GLN
1	D	208	HIS
1	D	243	ASN
1	D	269	ASN
1	D	282	GLN
1	D	388	ASN
1	E	4	ASN
1	E	18	ASN
1	E	21	ASN
1	E	33	ASN
1	E	36	HIS
1	E	67	GLN
1	E	150	HIS
1	E	165	GLN
1	E	208	HIS
1	E	243	ASN
1	E	269	ASN
1	E	282	GLN
1	E	388	ASN
1	F	21	ASN
1	F	33	ASN
1	F	165	GLN
1	F	208	HIS
1	F	226	ASN
1	F	269	ASN
1	F	282	GLN
1	F	388	ASN
1	G	21	ASN
1	G	33	ASN
1	G	35	ASN
1	G	165	GLN
1	G	208	HIS
1	G	226	ASN
1	G	243	ASN
1	G	282	GLN
1	G	388	ASN

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Mol	Chain	Res	Type
2	Y	45	HIS
2	Y	48	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
3	FAD	B	400	-	58,58,58	1.41	11 (18%)	85,89,89	1.71	18 (21%)
3	FAD	D	400	-	58,58,58	1.50	8 (13%)	85,89,89	1.85	24 (28%)
3	FAD	G	400	-	58,58,58	1.49	9 (15%)	85,89,89	1.64	17 (20%)
3	FAD	A	400	-	58,58,58	1.55	10 (17%)	85,89,89	1.85	24 (28%)
3	FAD	F	400	-	58,58,58	1.32	7 (12%)	85,89,89	1.76	19 (22%)
3	FAD	E	400	-	58,58,58	1.34	6 (10%)	85,89,89	1.71	20 (23%)

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
3	FAD	B	400	-	-	7/34/50/50	0/6/6/6
3	FAD	D	400	-	-	7/34/50/50	0/6/6/6
3	FAD	G	400	-	-	4/34/50/50	0/6/6/6
3	FAD	A	400	-	-	5/34/50/50	0/6/6/6
3	FAD	F	400	-	-	8/34/50/50	0/6/6/6
3	FAD	E	400	-	-	2/34/50/50	0/6/6/6

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	400	FAD	C4X-N5	5.79	1.43	1.30
3	D	400	FAD	C1'-C2'	5.07	1.59	1.52
3	D	400	FAD	C4X-N5	4.52	1.40	1.30
3	A	400	FAD	C2A-N3A	4.50	1.41	1.33
3	G	400	FAD	C1'-C2'	4.43	1.58	1.52
3	A	400	FAD	C1'-C2'	4.27	1.58	1.52
3	E	400	FAD	C4X-N5	4.24	1.39	1.30
3	E	400	FAD	PA-O3P	3.89	1.63	1.59
3	E	400	FAD	C1'-C2'	3.79	1.57	1.52
3	A	400	FAD	P-O3P	3.72	1.63	1.59
3	F	400	FAD	C4X-N5	3.72	1.38	1.30
3	B	400	FAD	C1'-C2'	3.67	1.57	1.52
3	A	400	FAD	C2A-N1A	3.58	1.40	1.33
3	D	400	FAD	C10-N1	3.44	1.40	1.33
3	F	400	FAD	C2A-N1A	3.40	1.40	1.33
3	B	400	FAD	P-O3P	-3.23	1.56	1.59
3	G	400	FAD	C8A-N7A	3.19	1.37	1.31
3	G	400	FAD	C8A-N9A	3.06	1.42	1.37
3	F	400	FAD	P-O3P	3.06	1.62	1.59
3	B	400	FAD	C10-N1	3.05	1.39	1.33
3	G	400	FAD	PA-O3P	2.97	1.62	1.59
3	G	400	FAD	C2A-N1A	2.97	1.39	1.33
3	A	400	FAD	C4X-N5	2.93	1.37	1.30
3	D	400	FAD	C2A-N1A	2.82	1.38	1.33
3	F	400	FAD	C1'-C2'	2.78	1.56	1.52
3	B	400	FAD	C4X-N5	2.77	1.36	1.30
3	B	400	FAD	C2A-N1A	2.77	1.38	1.33
3	B	400	FAD	C2A-N3A	2.59	1.38	1.33
3	F	400	FAD	C2A-N3A	2.52	1.38	1.33
3	D	400	FAD	PA-O2A	-2.49	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	400	FAD	C2A-N1A	2.49	1.38	1.33
3	A	400	FAD	P-O2P	-2.45	1.44	1.55
3	F	400	FAD	C8A-N7A	2.44	1.36	1.31
3	B	400	FAD	PA-O3P	2.39	1.62	1.59
3	G	400	FAD	C10-N1	2.37	1.38	1.33
3	B	400	FAD	C1'-N10	2.34	1.53	1.47
3	A	400	FAD	C10-N1	2.30	1.37	1.33
3	E	400	FAD	C2A-N3A	2.28	1.38	1.33
3	A	400	FAD	C5'-C4'	2.27	1.54	1.51
3	E	400	FAD	C1'-N10	2.25	1.53	1.47
3	G	400	FAD	C2A-N3A	2.20	1.37	1.33
3	D	400	FAD	C10-N10	2.20	1.42	1.37
3	B	400	FAD	O4B-C4B	-2.18	1.40	1.45
3	F	400	FAD	C5'-C4'	2.16	1.54	1.51
3	D	400	FAD	O4B-C1B	2.10	1.46	1.42
3	G	400	FAD	C1'-N10	2.09	1.52	1.47
3	B	400	FAD	C5A-N7A	-2.09	1.35	1.39
3	D	400	FAD	O4B-C4B	-2.06	1.40	1.45
3	B	400	FAD	C5'-C4'	2.01	1.54	1.51
3	A	400	FAD	C9-C9A	-2.01	1.36	1.39
3	A	400	FAD	C8A-N7A	2.01	1.35	1.31

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	FAD	N3A-C2A-N1A	-7.31	117.51	128.58
3	G	400	FAD	N3A-C2A-N1A	-6.34	118.99	128.58
3	F	400	FAD	N3A-C2A-N1A	-5.83	119.76	128.58
3	B	400	FAD	N3A-C2A-N1A	-5.67	120.00	128.58
3	D	400	FAD	N3A-C2A-N1A	-5.65	120.03	128.58
3	B	400	FAD	N9A-C8A-N7A	-5.14	106.64	113.94
3	E	400	FAD	N3A-C2A-N1A	-5.09	120.88	128.58
3	D	400	FAD	C4-N3-C2	-4.62	117.43	125.64
3	B	400	FAD	C5A-N7A-C8A	4.58	110.65	103.45
3	F	400	FAD	N9A-C8A-N7A	-4.49	107.57	113.94
3	A	400	FAD	N9A-C8A-N7A	-4.33	107.79	113.94
3	G	400	FAD	C9A-C5X-N5	-4.30	117.89	122.45
3	G	400	FAD	C5X-C9A-N10	4.29	121.85	117.97
3	D	400	FAD	N9A-C8A-N7A	-4.18	108.00	113.94
3	A	400	FAD	C4A-N9A-C8A	3.99	109.93	105.74
3	G	400	FAD	N9A-C8A-N7A	-3.95	108.33	113.94
3	E	400	FAD	N9A-C8A-N7A	-3.89	108.41	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	400	FAD	C5A-N7A-C8A	3.75	109.35	103.45
3	F	400	FAD	O4'-C4'-C3'	-3.71	100.56	109.25
3	E	400	FAD	C5A-C4A-N3A	-3.65	121.70	126.72
3	E	400	FAD	C5X-C9A-N10	3.64	121.25	117.97
3	A	400	FAD	O3'-C3'-C2'	3.62	117.14	108.93
3	E	400	FAD	O2A-PA-O3P	3.60	117.01	107.27
3	E	400	FAD	C4-N3-C2	-3.53	119.37	125.64
3	D	400	FAD	C10-N1-C2	3.51	124.44	116.85
3	D	400	FAD	C4X-C4-N3	3.47	122.09	113.25
3	E	400	FAD	C5A-N7A-C8A	3.41	108.81	103.45
3	F	400	FAD	O3P-P-O1P	-3.41	100.46	110.70
3	F	400	FAD	C4X-C10-N10	3.35	121.27	116.48
3	D	400	FAD	C5A-N7A-C8A	3.34	108.69	103.45
3	B	400	FAD	C9A-C5X-N5	-3.30	118.95	122.45
3	D	400	FAD	O4-C4-C4X	-3.25	117.95	126.53
3	D	400	FAD	O3'-C3'-C2'	3.23	116.28	108.93
3	F	400	FAD	C5A-C4A-N3A	-3.23	122.27	126.72
3	F	400	FAD	O3'-C3'-C4'	-3.17	101.72	108.93
3	G	400	FAD	C2A-N3A-C4A	3.10	119.40	111.83
3	B	400	FAD	O4'-C4'-C3'	-3.09	102.02	109.25
3	F	400	FAD	C2A-N3A-C4A	3.05	119.27	111.83
3	A	400	FAD	C5A-N7A-C8A	3.04	108.23	103.45
3	G	400	FAD	C5A-C4A-N3A	-3.02	122.56	126.72
3	D	400	FAD	O2'-C2'-C1'	3.02	122.61	110.20
3	E	400	FAD	C1'-C2'-C3'	3.02	117.84	109.66
3	F	400	FAD	O3'-C3'-C2'	3.00	115.75	108.93
3	A	400	FAD	C9A-C5X-N5	-3.00	119.27	122.45
3	B	400	FAD	O2'-C2'-C1'	2.99	122.51	110.20
3	F	400	FAD	O2'-C2'-C3'	2.98	116.22	109.25
3	A	400	FAD	O2'-C2'-C1'	2.97	122.42	110.20
3	D	400	FAD	C4X-C10-N1	-2.97	117.31	124.59
3	F	400	FAD	C10-C4X-N5	-2.95	118.79	124.81
3	A	400	FAD	O4'-C4'-C3'	-2.95	102.35	109.25
3	B	400	FAD	C4-N3-C2	-2.86	120.56	125.64
3	E	400	FAD	C4X-C10-N10	2.85	120.56	116.48
3	D	400	FAD	C2A-N3A-C4A	2.85	118.78	111.83
3	D	400	FAD	C4'-C3'-C2'	-2.80	108.91	113.57
3	A	400	FAD	C10-C4X-N5	-2.79	119.11	124.81
3	F	400	FAD	O2A-PA-O3P	2.78	114.78	107.27
3	B	400	FAD	C4-C4X-C10	2.76	121.66	116.93
3	A	400	FAD	N6A-C6A-N1A	2.74	124.48	118.38
3	E	400	FAD	C2A-N3A-C4A	2.74	118.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	400	FAD	C4-N3-C2	-2.73	120.80	125.64
3	B	400	FAD	C4A-C5A-N7A	-2.73	107.47	110.58
3	D	400	FAD	C10-C4X-N5	-2.71	119.27	124.81
3	E	400	FAD	C4X-C4-N3	2.70	120.13	113.25
3	E	400	FAD	C4X-C10-N1	-2.69	117.98	124.59
3	D	400	FAD	C5A-C4A-N3A	-2.68	123.02	126.72
3	D	400	FAD	C4A-N9A-C8A	2.68	108.55	105.74
3	A	400	FAD	C2A-N1A-C6A	2.68	123.13	118.73
3	A	400	FAD	C4X-C10-N10	2.68	120.31	116.48
3	A	400	FAD	C2A-N3A-C4A	2.67	118.36	111.83
3	B	400	FAD	C10-C4X-N5	-2.65	119.40	124.81
3	D	400	FAD	C9A-C5X-N5	-2.63	119.66	122.45
3	E	400	FAD	N3A-C4A-N9A	2.63	131.63	127.17
3	A	400	FAD	C5A-C4A-N3A	-2.62	123.11	126.72
3	A	400	FAD	C6-C5X-C9A	2.59	122.61	119.05
3	A	400	FAD	O3B-C3B-C4B	-2.58	103.66	111.08
3	B	400	FAD	C4A-N9A-C1B	-2.57	120.63	126.63
3	B	400	FAD	C5X-N5-C4X	2.56	122.23	118.09
3	A	400	FAD	C6A-C5A-C4A	2.54	120.64	117.18
3	A	400	FAD	C4A-N9A-C1B	-2.53	120.72	126.63
3	F	400	FAD	C4A-C5A-N7A	-2.51	107.71	110.58
3	B	400	FAD	C4A-N9A-C8A	2.51	108.37	105.74
3	A	400	FAD	N3A-C4A-N9A	2.50	131.41	127.17
3	D	400	FAD	C4X-C10-N10	2.48	120.04	116.48
3	G	400	FAD	C4X-C4-N3	2.46	119.52	113.25
3	G	400	FAD	C4-N3-C2	-2.43	121.32	125.64
3	F	400	FAD	C4-C4X-N5	2.42	121.56	118.21
3	E	400	FAD	C4-C4X-C10	2.42	121.08	116.93
3	G	400	FAD	C9-C9A-N10	-2.42	118.61	121.85
3	B	400	FAD	C5A-C4A-N3A	-2.37	123.45	126.72
3	B	400	FAD	C2A-N1A-C6A	2.35	122.59	118.73
3	D	400	FAD	C5B-C4B-C3B	-2.33	106.81	115.21
3	B	400	FAD	C2A-N3A-C4A	2.33	117.52	111.83
3	E	400	FAD	C9A-C5X-N5	-2.33	119.98	122.45
3	A	400	FAD	C5X-N5-C4X	2.33	121.85	118.09
3	E	400	FAD	C10-C4X-N5	-2.29	120.12	124.81
3	G	400	FAD	C4A-N9A-C8A	2.29	108.14	105.74
3	A	400	FAD	C5A-C6A-N6A	-2.27	117.67	123.29
3	E	400	FAD	C6-C5X-C9A	2.26	122.16	119.05
3	A	400	FAD	C5X-C6-C7	-2.26	116.63	120.83
3	G	400	FAD	C2A-N1A-C6A	2.25	122.43	118.73
3	G	400	FAD	C5A-N7A-C8A	2.23	106.96	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	400	FAD	O2'-C2'-C1'	2.22	119.31	110.20
3	A	400	FAD	C4X-C10-N1	-2.20	119.20	124.59
3	F	400	FAD	C9A-C5X-N5	-2.20	120.12	122.45
3	G	400	FAD	C8M-C8-C9	-2.18	115.74	119.57
3	F	400	FAD	C4A-N9A-C8A	2.17	108.01	105.74
3	F	400	FAD	O3B-C3B-C4B	-2.16	104.87	111.08
3	D	400	FAD	O2A-PA-O3P	2.16	113.11	107.27
3	D	400	FAD	C5X-C9A-N10	2.16	119.92	117.97
3	D	400	FAD	O2P-P-O5'	2.14	117.28	107.57
3	D	400	FAD	N3A-C4A-N9A	2.14	130.80	127.17
3	E	400	FAD	C7M-C7-C6	-2.11	115.86	119.57
3	A	400	FAD	O2'-C2'-C3'	2.10	114.17	109.25
3	D	400	FAD	O2B-C2B-C1B	2.09	117.31	110.10
3	E	400	FAD	C4A-C5A-N7A	-2.08	108.21	110.58
3	G	400	FAD	C4-C4X-N5	2.07	121.07	118.21
3	B	400	FAD	C4X-C10-N10	2.07	119.44	116.48
3	G	400	FAD	C6-C5X-C9A	2.06	121.88	119.05
3	G	400	FAD	O4-C4-C4X	-2.05	121.12	126.53
3	B	400	FAD	C8M-C8-C9	-2.04	115.98	119.57
3	D	400	FAD	C2A-N1A-C6A	2.03	122.06	118.73
3	E	400	FAD	C4A-N9A-C8A	2.02	107.86	105.74

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	FAD	C1'-C2'-C3'-O3'
3	A	400	FAD	C1'-C2'-C3'-C4'
3	A	400	FAD	O4'-C4'-C5'-O5'
3	B	400	FAD	C2'-C1'-N10-C10
3	B	400	FAD	C1'-C2'-C3'-O3'
3	B	400	FAD	C1'-C2'-C3'-C4'
3	D	400	FAD	C1'-C2'-C3'-O3'
3	D	400	FAD	C1'-C2'-C3'-C4'
3	D	400	FAD	O4'-C4'-C5'-O5'
3	E	400	FAD	C2'-C1'-N10-C10
3	F	400	FAD	C2'-C1'-N10-C10
3	F	400	FAD	C1'-C2'-C3'-C4'
3	G	400	FAD	C1'-C2'-C3'-C4'
3	A	400	FAD	O3'-C3'-C4'-O4'
3	F	400	FAD	O3'-C3'-C4'-O4'
3	F	400	FAD	O4'-C4'-C5'-O5'

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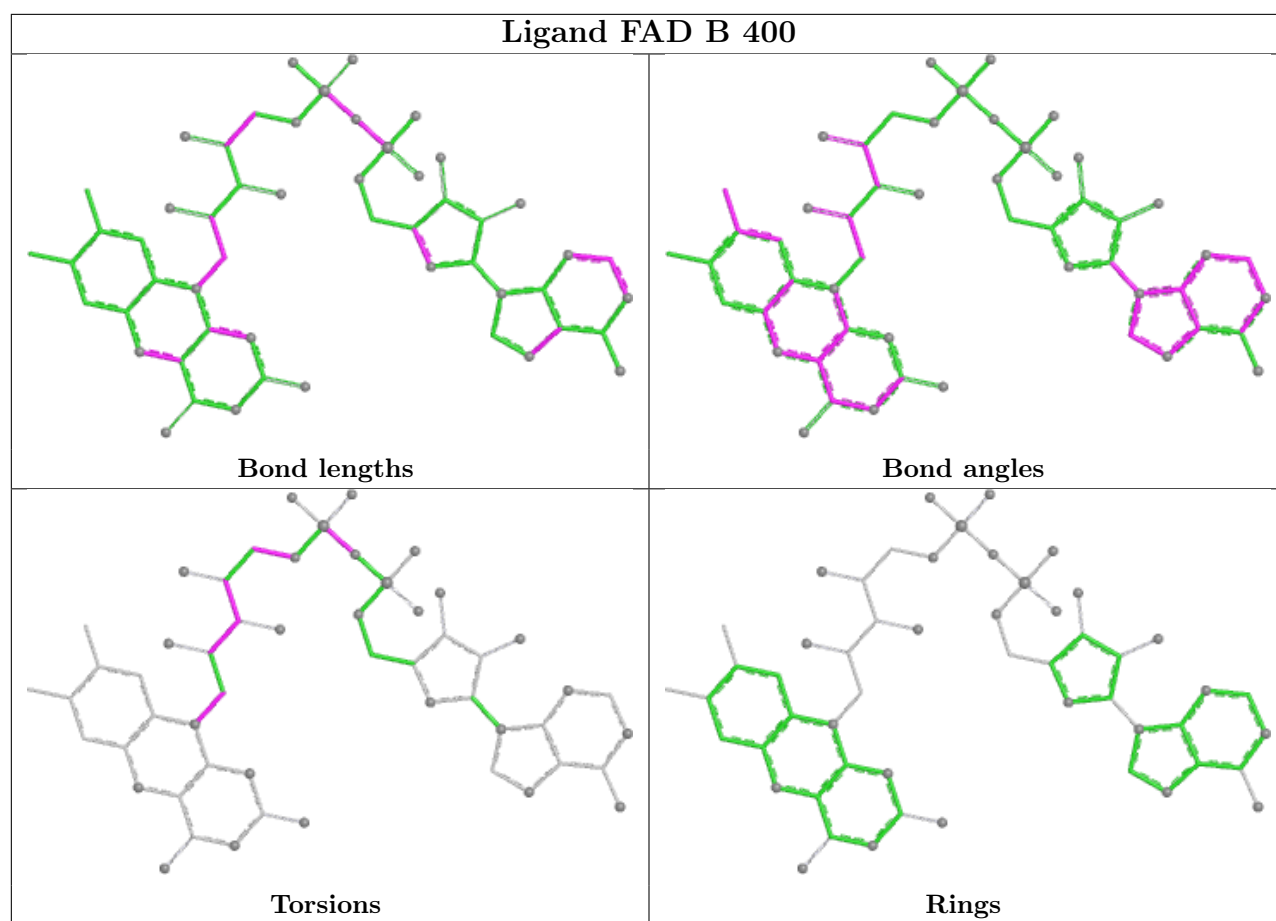
Mol	Chain	Res	Type	Atoms
3	A	400	FAD	O3'-C3'-C4'-C5'
3	D	400	FAD	O3'-C3'-C4'-C5'
3	D	400	FAD	O3'-C3'-C4'-O4'
3	F	400	FAD	O3'-C3'-C4'-C5'
3	F	400	FAD	C2'-C3'-C4'-O4'
3	B	400	FAD	PA-O3P-P-O5'
3	D	400	FAD	PA-O3P-P-O5'
3	G	400	FAD	PA-O3P-P-O5'
3	G	400	FAD	C1'-C2'-C3'-O3'
3	D	400	FAD	C4'-C5'-O5'-P
3	B	400	FAD	O3'-C3'-C4'-O4'
3	F	400	FAD	PA-O3P-P-O5'
3	B	400	FAD	C4'-C5'-O5'-P
3	G	400	FAD	C4'-C5'-O5'-P
3	B	400	FAD	O3'-C3'-C4'-C5'
3	F	400	FAD	C2'-C3'-C4'-C5'
3	E	400	FAD	C4'-C5'-O5'-P

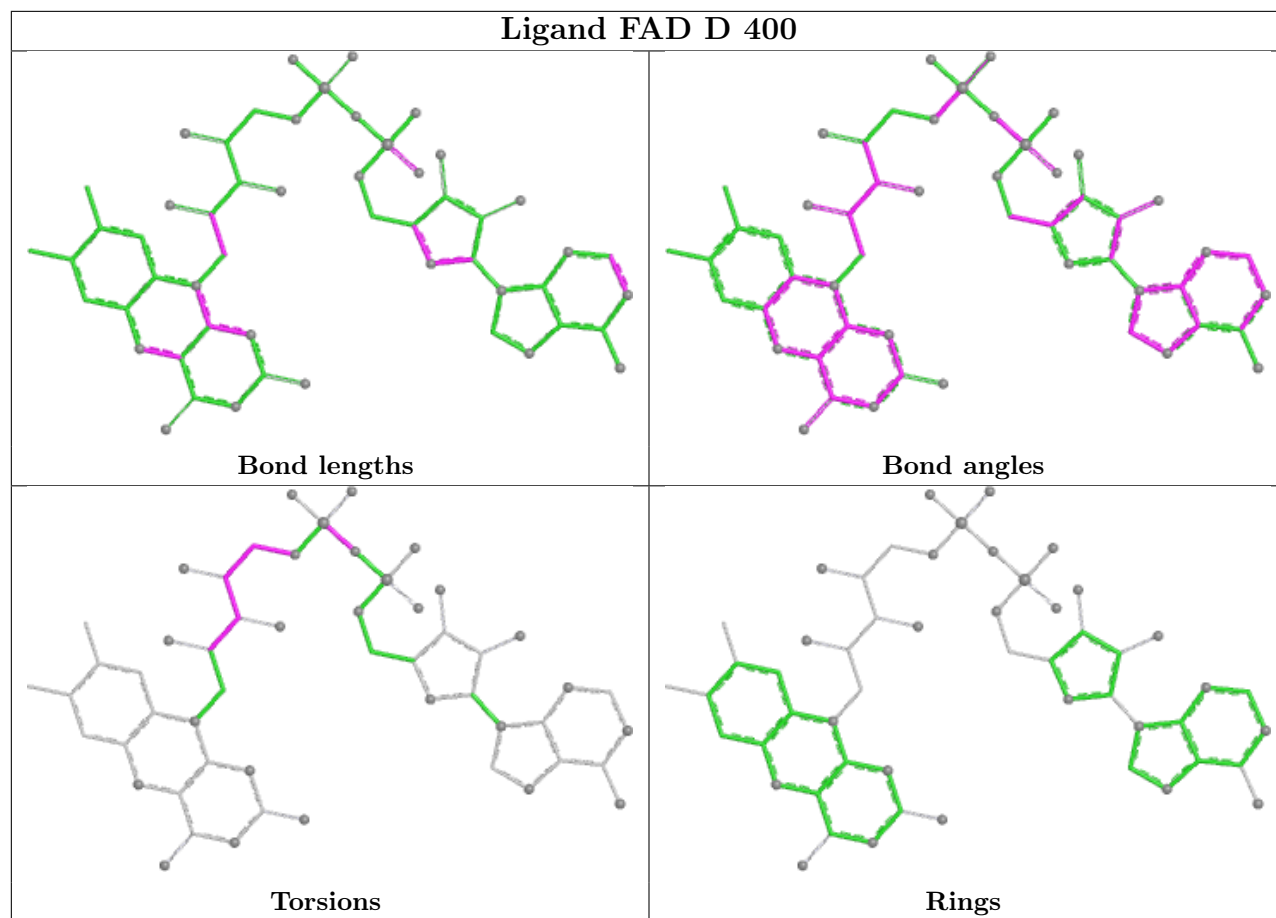
There are no ring outliers.

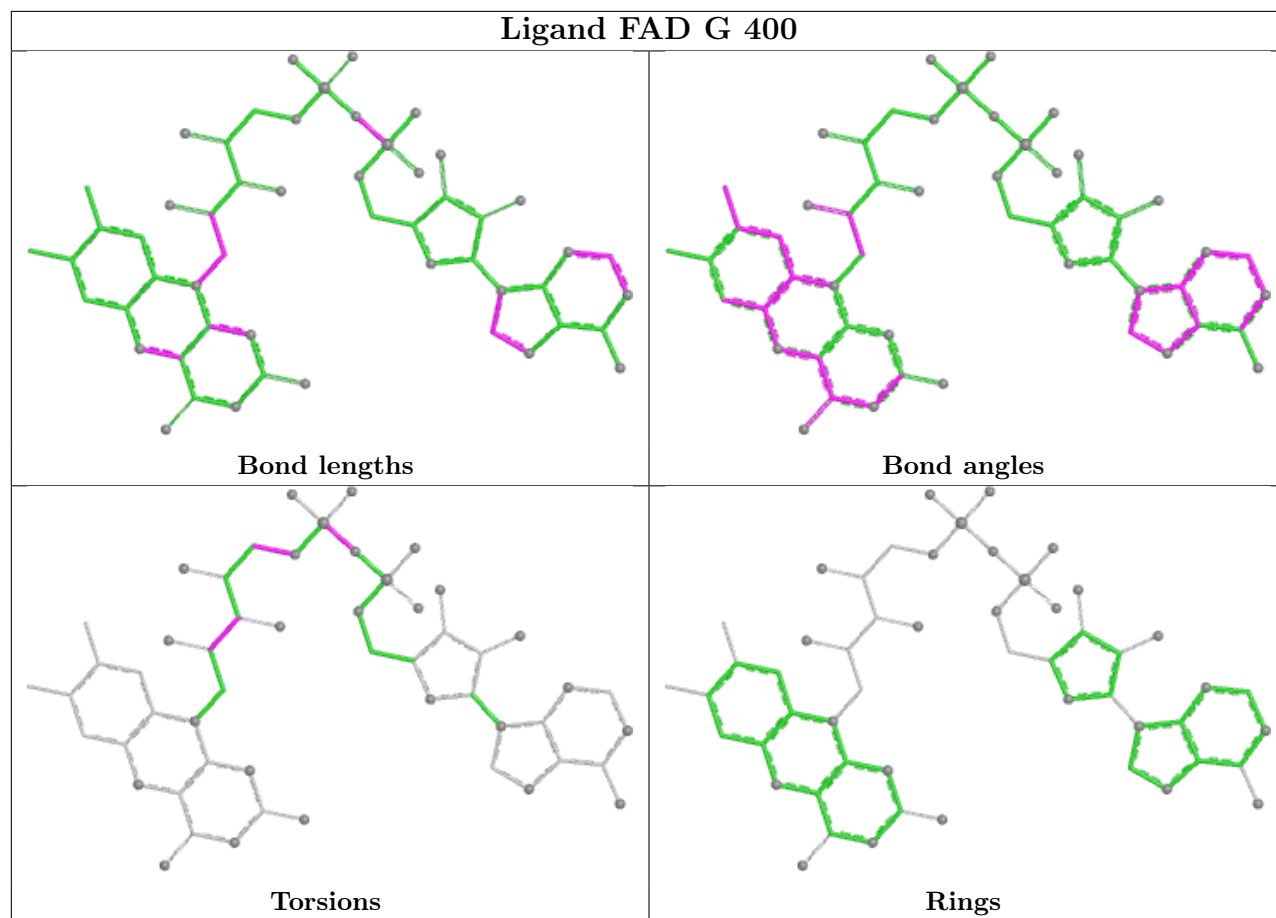
6 monomers are involved in 26 short contacts:

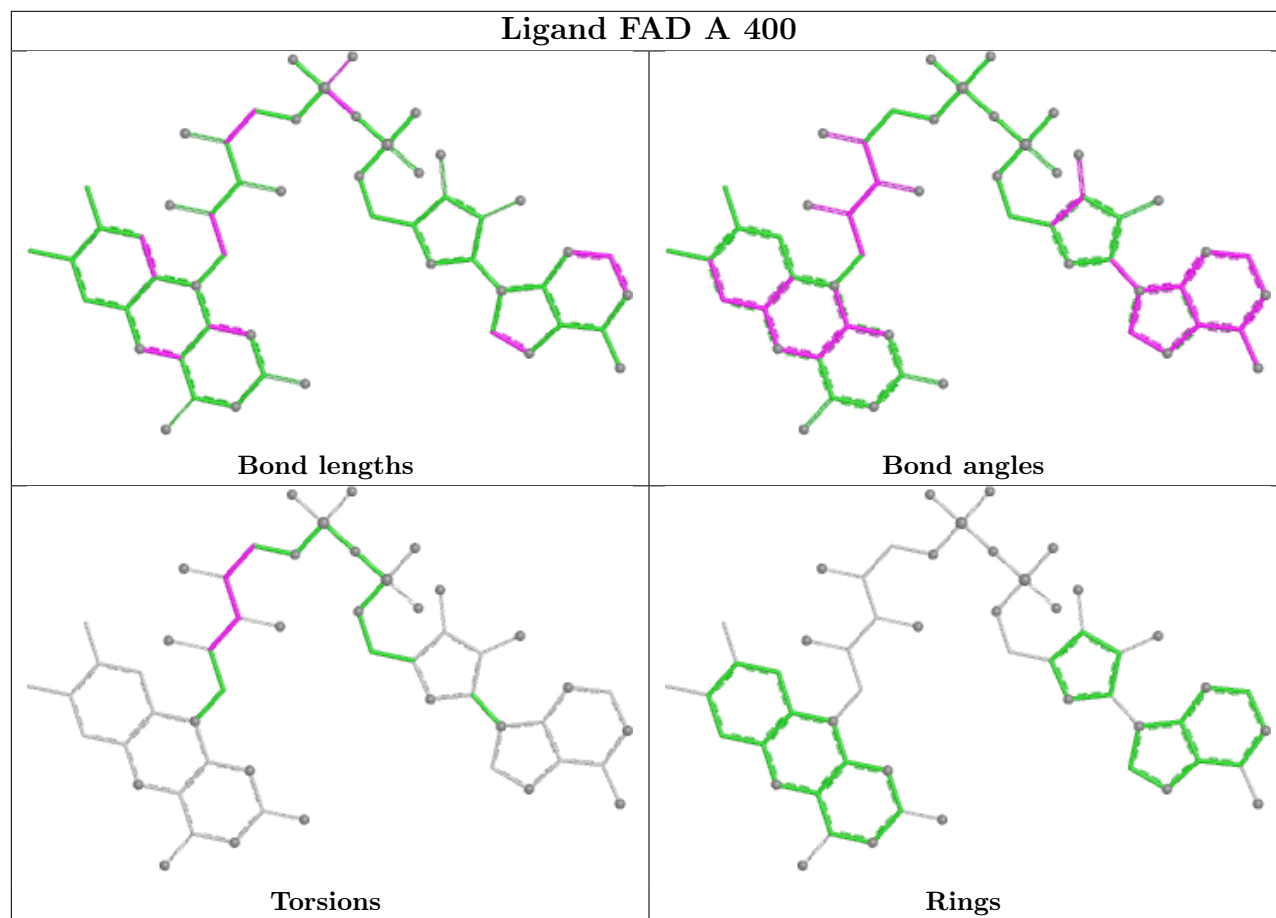
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	FAD	4	0
3	D	400	FAD	5	0
3	G	400	FAD	4	0
3	A	400	FAD	4	0
3	F	400	FAD	5	0
3	E	400	FAD	4	0

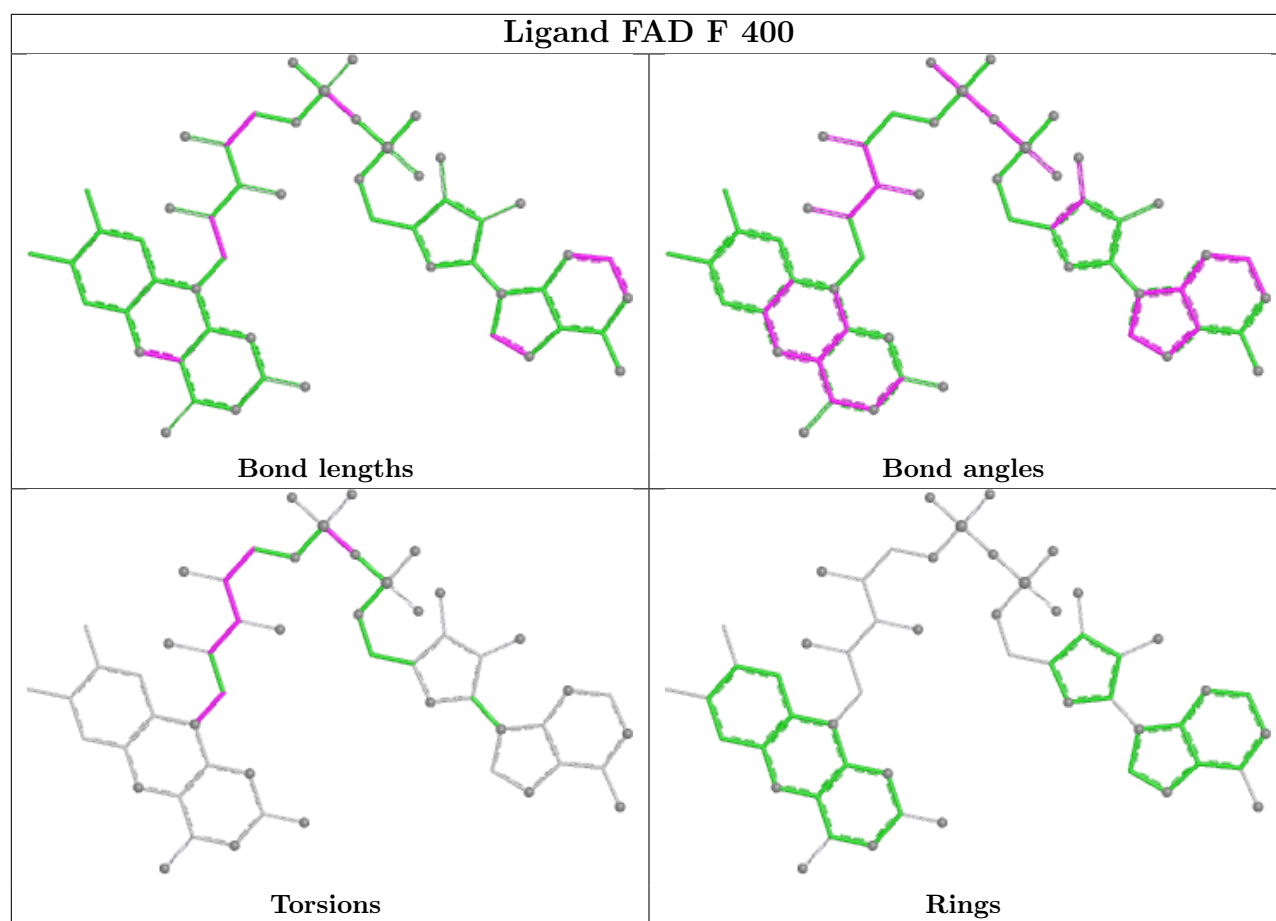
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

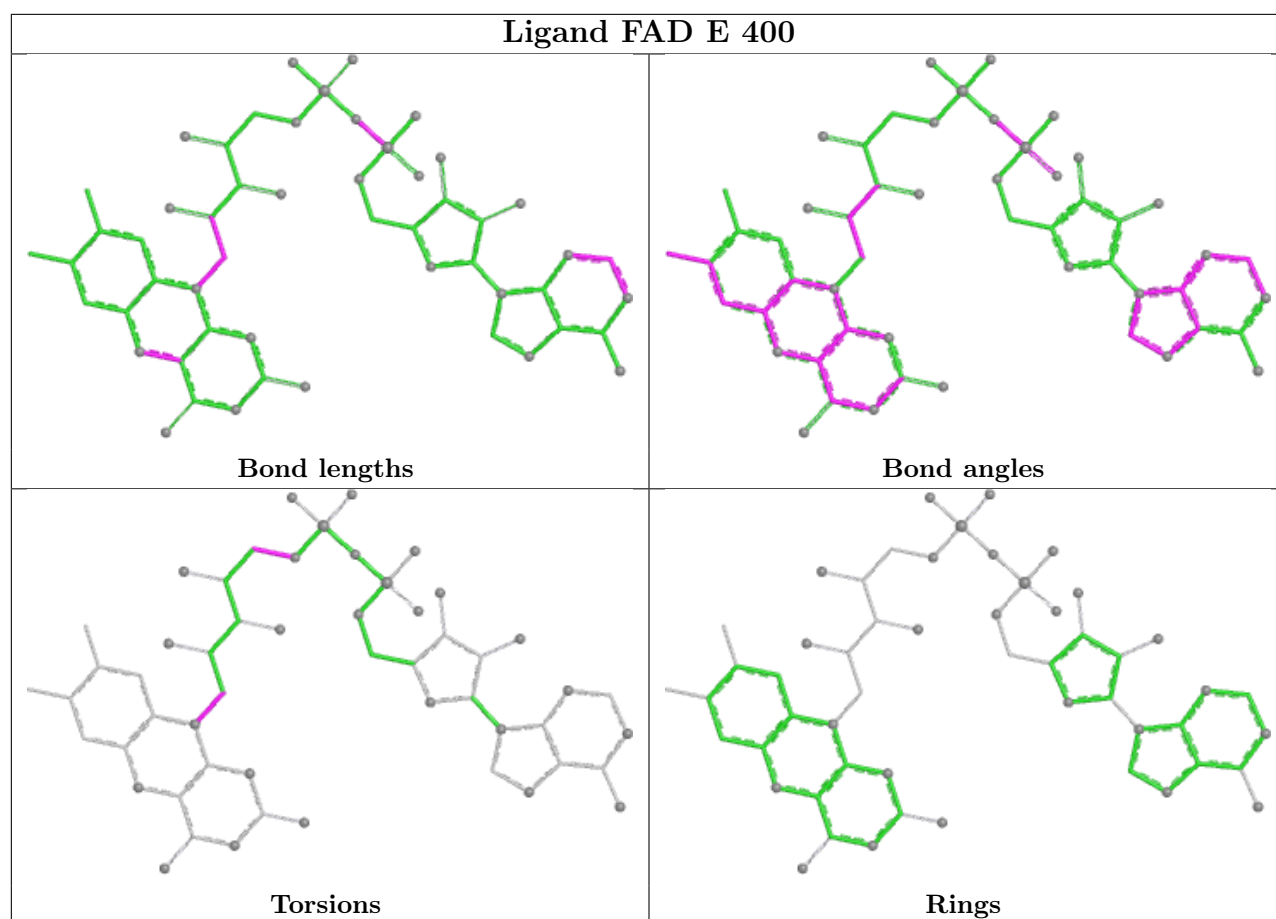












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/397 (97%)	-0.25	0 100 100	13, 25, 43, 57	2 (0%)
1	B	393/397 (98%)	-0.13	5 (1%) 75 77	13, 27, 48, 92	2 (0%)
1	D	390/397 (98%)	1.50	122 (31%) 1 1	23, 47, 75, 88	2 (0%)
1	E	391/397 (98%)	1.49	145 (37%) 1 1	18, 51, 99, 141	1 (0%)
1	F	390/397 (98%)	0.03	3 (0%) 82 84	16, 31, 50, 64	2 (0%)
1	G	389/397 (97%)	0.64	22 (5%) 29 31	22, 39, 61, 77	0
2	Y	8/8 (100%)	1.43	4 (50%) 0 0	29, 48, 58, 76	0
All	All	2350/2390 (98%)	0.55	301 (12%) 7 8	13, 35, 73, 141	9 (0%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	151	TRP	6.9
1	E	144	ALA	6.5
1	E	188	VAL	6.1
1	E	223	PRO	6.0
1	E	227	ILE	5.7
1	E	108	ALA	5.6
1	E	220	VAL	5.6
1	E	222	VAL	5.5
1	E	195	PRO	5.3
1	E	152	LEU	5.3
1	E	216	PHE	5.2
1	E	189	ILE	5.1
1	E	109	LEU	5.1
1	E	153	LEU	4.9
1	E	197	ILE	4.7
1	E	178	ALA	4.7
1	E	187	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	196	GLY	4.6
1	E	194	PHE	4.6
1	E	221	LYS	4.5
1	D	113	TYR	4.4
1	E	150	HIS	4.4
1	E	193	ASN	4.4
1	E	169	LEU	4.4
1	E	228	LEU	4.4
1	D	49	LEU	4.3
1	E	148	GLY	4.3
1	E	173	ALA	4.3
1	D	50	GLY	4.3
1	E	113	TYR	4.2
1	G	68	GLY	4.2
1	E	170	ILE	4.2
1	D	351	TYR	4.2
1	E	122	PHE	4.2
1	E	226	ASN	4.2
1	E	149	ASP	4.1
1	E	231	PRO	4.1
1	E	217	LEU	4.0
1	D	108	ALA	4.0
1	E	174	TYR	4.0
1	E	139	ALA	3.9
1	D	53	GLY	3.8
1	D	61	GLY	3.8
1	E	164	ALA	3.8
1	E	177	LYS	3.8
1	D	45	PRO	3.8
1	D	123	LEU	3.8
1	D	60	TYR	3.7
1	E	171	TYR	3.7
1	E	123	LEU	3.7
1	D	25	VAL	3.7
1	E	118	SER	3.7
1	E	184	LEU	3.7
1	E	215	LEU	3.7
1	D	11	MET	3.7
1	D	122	PHE	3.7
1	E	147	LYS	3.7
1	D	5	LEU	3.6
1	D	223	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	175	THR	3.6
1	E	60	TYR	3.6
1	E	146	ASP	3.5
1	E	213	GLY	3.5
1	E	229	GLY	3.5
1	E	224	LYS	3.5
1	D	74	ILE	3.5
1	E	141	SER	3.4
1	E	143	THR	3.4
1	D	119	SER	3.4
1	E	106	SER	3.4
1	D	65	MET	3.3
1	E	198	LYS	3.3
1	E	155	GLY	3.3
1	E	180	GLY	3.3
1	E	391	GLY	3.3
1	D	151	TRP	3.3
1	E	225	GLU	3.3
1	E	39	TYR	3.3
1	E	166	ALA	3.3
1	E	186	ALA	3.3
1	D	19	PHE	3.3
1	G	66	ASP	3.3
1	E	64	GLY	3.3
1	E	199	THR	3.2
1	D	105	GLY	3.2
1	D	353	VAL	3.2
1	E	101	ILE	3.2
1	D	12	LEU	3.2
1	E	117	LEU	3.2
1	E	97	CYS	3.2
1	D	16	VAL	3.2
1	E	179	ALA	3.2
1	E	90	LEU	3.2
1	E	61	GLY	3.2
1	D	117	LEU	3.1
1	E	176	ASP	3.1
1	E	104	TYR	3.1
1	D	51	PHE	3.1
1	D	118	SER	3.1
1	E	200	SER	3.1
1	E	168	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	159	TRP	3.1
1	D	64	GLY	3.1
1	D	96	GLY	3.1
1	E	98	ALA	3.1
1	D	70	LEU	3.1
1	D	227	ILE	3.1
1	E	212	THR	3.0
1	E	167	ASP	3.0
1	D	109	LEU	3.0
1	E	133	ALA	3.0
1	D	106	SER	3.0
1	D	275	GLY	3.0
1	E	158	THR	3.0
1	E	57	PRO	3.0
1	E	102	LEU	3.0
1	E	183	GLY	3.0
1	E	103	THR	3.0
1	E	235	ALA	2.9
1	D	43	VAL	2.9
1	E	56	ILE	2.9
1	E	237	ILE	2.9
1	E	99	TYR	2.9
1	G	351	TYR	2.9
1	D	14	LYS	2.9
1	E	105	GLY	2.9
1	D	55	VAL	2.9
1	D	222	VAL	2.9
1	E	163	ALA	2.9
1	D	115	PRO	2.8
1	E	52	PHE	2.8
2	Y	42	GLY	2.8
1	E	219	ASN	2.8
1	D	148	GLY	2.8
1	E	53	GLY	2.8
1	E	40	GLU	2.8
1	G	308	ALA	2.8
1	D	9	LEU	2.8
1	E	160	ILE	2.8
1	D	44	ARG	2.8
2	Y	47	HIS	2.8
1	G	64	GLY	2.8
1	D	42	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	306	ALA	2.8
1	D	57	PRO	2.8
1	D	75	VAL	2.8
1	E	192	ARG	2.7
1	E	35	ASN	2.7
1	B	393	HIS	2.7
1	D	66	ASP	2.7
1	D	356	PHE	2.7
1	E	112	LYS	2.7
1	E	120	ALA	2.7
1	D	114	VAL	2.7
1	D	59	GLU	2.7
1	D	54	THR	2.7
1	E	190	GLU	2.7
1	D	56	ILE	2.7
1	D	52	PHE	2.7
1	D	152	LEU	2.7
1	D	72	ALA	2.6
1	D	102	LEU	2.6
1	E	49	LEU	2.6
1	G	65	MET	2.6
1	E	191	PRO	2.6
1	E	185	SER	2.6
1	D	24	ILE	2.6
1	E	100	THR	2.6
1	D	20	VAL	2.6
1	E	119	SER	2.6
1	E	114	VAL	2.6
1	G	67	GLN	2.6
1	E	107	GLU	2.6
1	E	140	MET	2.6
1	D	193	ASN	2.6
1	E	154	ASN	2.6
1	E	142	SER	2.6
1	E	55	VAL	2.5
1	G	114	VAL	2.5
1	D	39	TYR	2.5
1	D	18	ASN	2.5
1	D	100	THR	2.5
1	E	165	GLN	2.5
1	D	220	VAL	2.5
1	E	172	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	2	ASP	2.5
1	D	62	GLY	2.5
1	G	389	ARG	2.5
1	F	108	ALA	2.5
1	D	112	LYS	2.5
1	E	37	PHE	2.5
1	G	151	TRP	2.5
1	D	76	THR	2.4
1	E	161	SER	2.4
1	D	277	PRO	2.4
1	D	23	LYS	2.4
1	D	314	LEU	2.4
1	D	37	PHE	2.4
1	D	47	GLY	2.4
1	E	126	PHE	2.4
1	E	218	ASP	2.4
1	D	86	LEU	2.4
1	E	145	GLU	2.4
1	D	7	LYS	2.4
1	D	17	ARG	2.4
1	E	45	PRO	2.4
1	E	42	ALA	2.4
1	B	391	GLY	2.4
1	G	385	ARG	2.4
1	D	199	THR	2.4
1	D	98	ALA	2.3
1	G	178	ALA	2.3
1	D	90	LEU	2.3
1	E	202	LEU	2.3
1	E	241	SER	2.3
2	Y	43	HIS	2.3
1	D	225	GLU	2.3
1	G	1	MET	2.3
1	D	27	PHE	2.3
1	E	43	VAL	2.3
1	D	267	TYR	2.3
1	D	343	GLY	2.3
1	E	44	ARG	2.3
1	D	22	LYS	2.3
1	G	3	PHE	2.3
1	E	94	VAL	2.3
1	E	129	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	71	ALA	2.3
1	D	120	ALA	2.3
1	D	166	ALA	2.3
1	E	127	GLY	2.3
1	E	214	GLU	2.2
1	D	3	PHE	2.2
1	D	101	ILE	2.2
1	D	111	LYS	2.2
1	D	1	MET	2.2
1	D	164	ALA	2.2
1	D	69	TRP	2.2
1	D	126	PHE	2.2
1	D	187	PHE	2.2
1	D	124	GLY	2.2
1	D	312	GLY	2.2
1	E	124	GLY	2.2
1	E	125	GLY	2.2
1	D	121	GLU	2.2
1	D	163	ALA	2.2
1	D	268	CYS	2.2
1	E	351	TYR	2.2
1	D	162	ASN	2.2
1	D	269	ASN	2.2
1	E	128	ILE	2.2
1	E	88	VAL	2.2
1	E	36	HIS	2.2
1	D	390	LYS	2.2
1	E	131	PRO	2.1
1	D	58	GLU	2.1
1	D	107	GLU	2.1
1	G	384	VAL	2.1
1	G	53	GLY	2.1
1	G	307	ALA	2.1
1	G	12	LEU	2.1
1	E	110	LYS	2.1
1	E	132	ASP	2.1
1	D	352	PRO	2.1
1	D	194	PHE	2.1
1	D	94	VAL	2.1
1	D	168	VAL	2.1
1	D	232	GLY	2.1
1	E	232	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	264	ALA	2.1
1	B	177[A]	LYS	2.1
1	G	60	TYR	2.1
1	D	197	ILE	2.1
1	D	274	PHE	2.1
1	E	23	LYS	2.1
1	E	95	LEU	2.1
1	D	13	GLN	2.1
1	B	351	TYR	2.1
1	D	150	HIS	2.1
1	G	312	GLY	2.1
1	E	111	LYS	2.1
1	E	116	LYS	2.1
1	B	48	GLU	2.0
1	F	152	LEU	2.0
1	E	201	ASN	2.0
1	E	310	ASP	2.0
2	Y	48	HIS	2.0
1	D	103	THR	2.0
1	D	349	THR	2.0
1	E	115	PRO	2.0
1	D	68	GLY	2.0
1	E	68	GLY	2.0
1	F	113	TYR	2.0
1	D	6	SER	2.0
1	D	207	SER	2.0
1	D	302	ALA	2.0
1	G	69	TRP	2.0
1	G	108	ALA	2.0
1	D	95	LEU	2.0
1	E	182	ARG	2.0
1	D	303	TYR	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

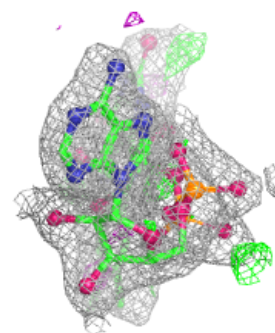
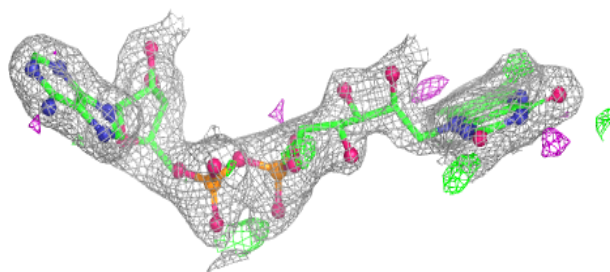
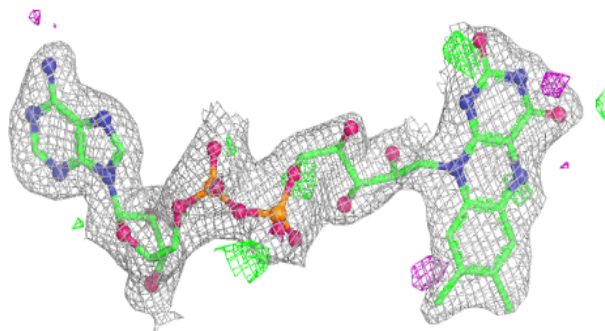
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	E	401	1/1	0.84	0.18	54,54,54,54	0
4	CL	D	401	1/1	0.90	0.11	45,45,45,45	0
3	FAD	E	400	53/53	0.90	0.11	32,43,55,62	0
3	FAD	D	400	53/53	0.95	0.07	21,27,37,39	0
3	FAD	G	400	53/53	0.95	0.07	24,29,35,36	0
3	FAD	B	400	53/53	0.96	0.06	15,20,25,26	0
4	CL	B	401	1/1	0.97	0.05	32,32,32,32	0
3	FAD	F	400	53/53	0.97	0.06	19,23,28,32	0
3	FAD	A	400	53/53	0.97	0.06	16,20,24,27	0
4	CL	G	401	1/1	0.97	0.05	38,38,38,38	0
4	CL	F	401	1/1	0.98	0.09	36,36,36,36	0
4	CL	A	401	1/1	0.98	0.05	32,32,32,32	0

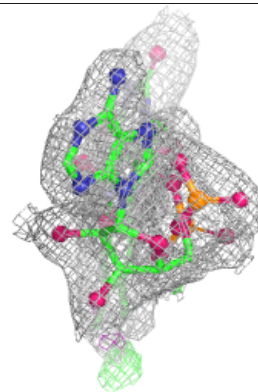
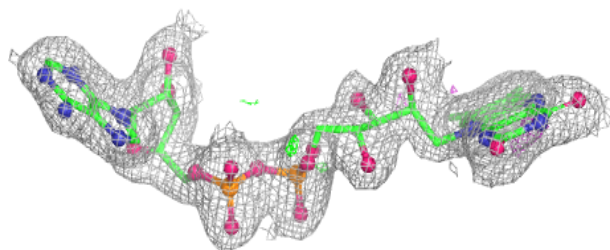
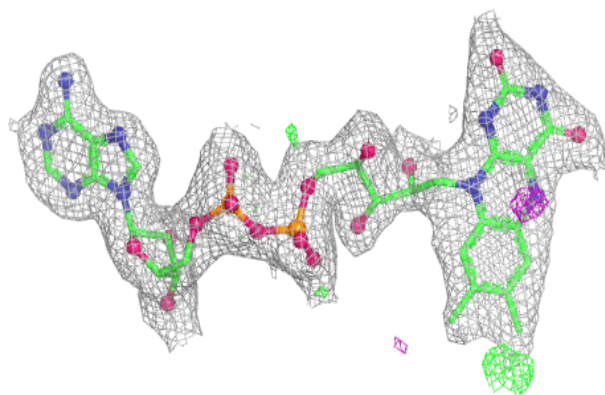
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD E 400:

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

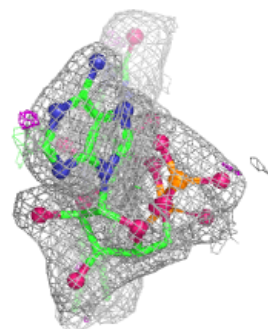
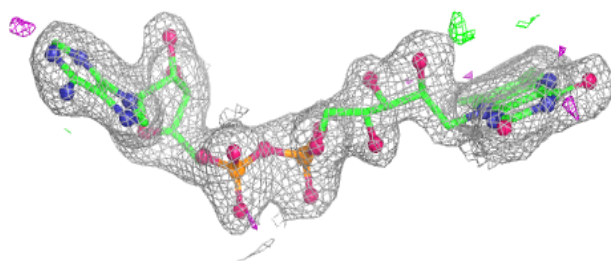
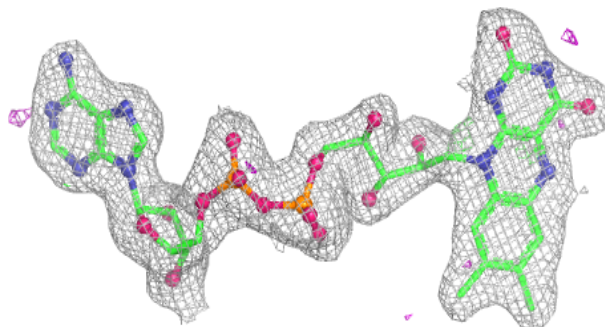
**Electron density around FAD D 400:**

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

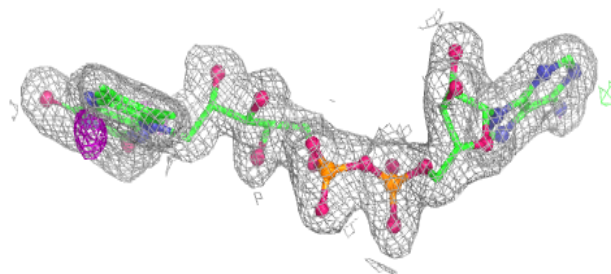
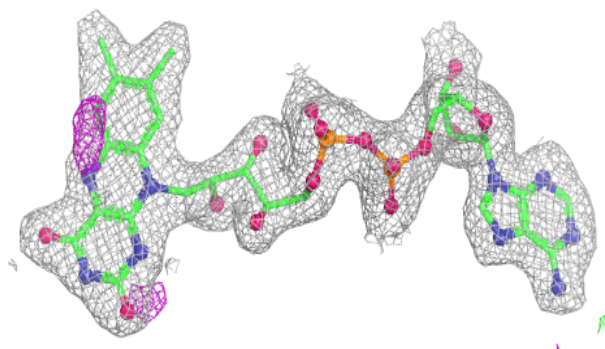


Electron density around FAD G 400:

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

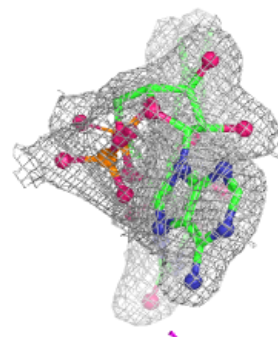
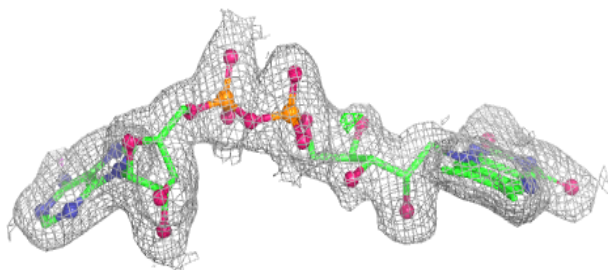
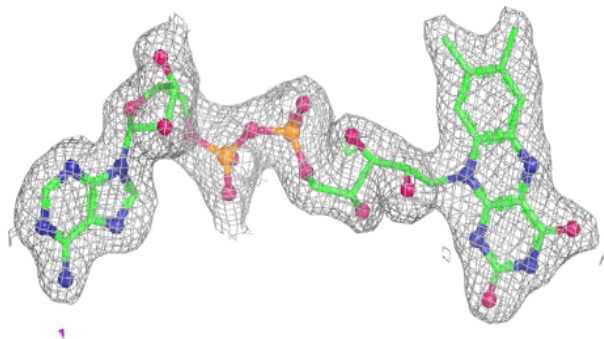
**Electron density around FAD B 400:**

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

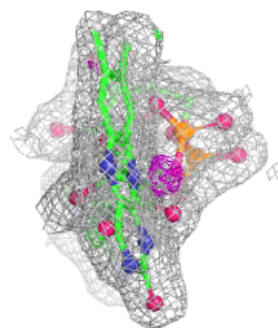
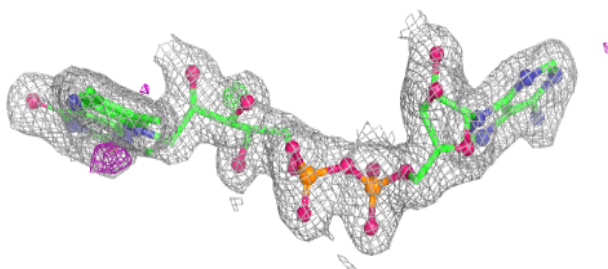
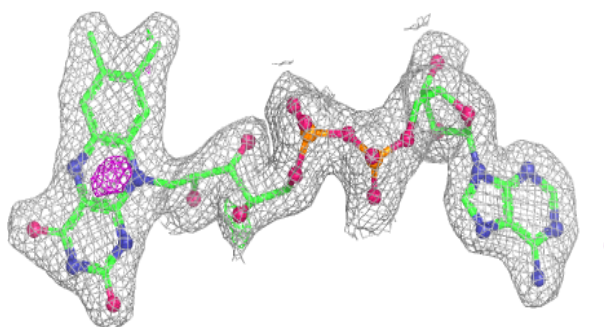


Electron density around FAD F 400:

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

**Electron density around FAD A 400:**

$2mF_o - DF_c$ (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.