



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2021 – 02:05 PM EDT

PDB ID : 6XBC  
Title : Crystal structure of Streptomyces sviveus SsDesB  
Authors : Lountos, G.T.; Giddings, L.A.; Waugh, D.S.  
Deposited on : 2020-06-05  
Resolution : 2.86 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](mailto: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.

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

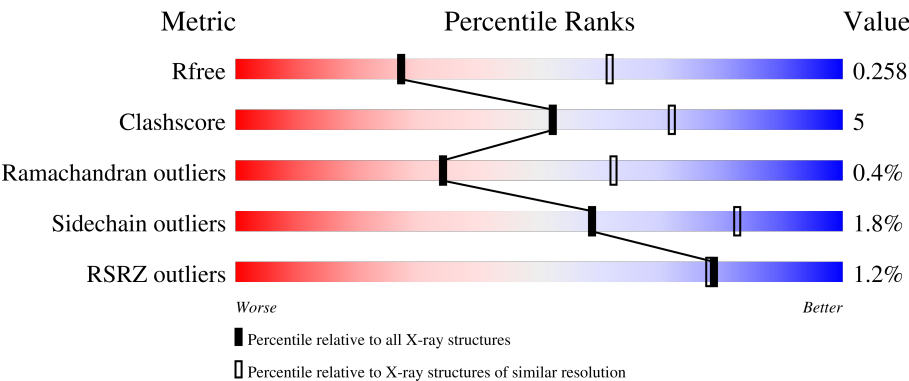
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.86 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 <sub>free</sub>	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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  $\geq 3$ , 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	425	<div><div></div><div>86%12%.</div></div>
1	B	425	<div><div>%</div><div>83%15%.</div></div>
1	C	425	<div><div>2%</div><div>85%12%.</div></div>
1	D	425	<div><div>2%</div><div>76%21%..</div></div>
1	E	425	<div><div>%</div><div>87%11%.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	425	
1	G	425	
1	H	425	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27122 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 Monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3340	2138	552	642	8			
1	B	416	Total	C	N	O	S	0	0	0
			3340	2138	552	642	8			
1	C	414	Total	C	N	O	S	0	0	0
			3326	2129	550	639	8			
1	D	414	Total	C	N	O	S	0	0	0
			3326	2129	550	639	8			
1	E	416	Total	C	N	O	S	0	0	0
			3340	2138	552	642	8			
1	F	415	Total	C	N	O	S	0	0	0
			3333	2134	551	640	8			
1	G	418	Total	C	N	O	S	0	0	0
			3353	2146	554	645	8			
1	H	416	Total	C	N	O	S	0	0	0
			3340	2138	552	642	8			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).




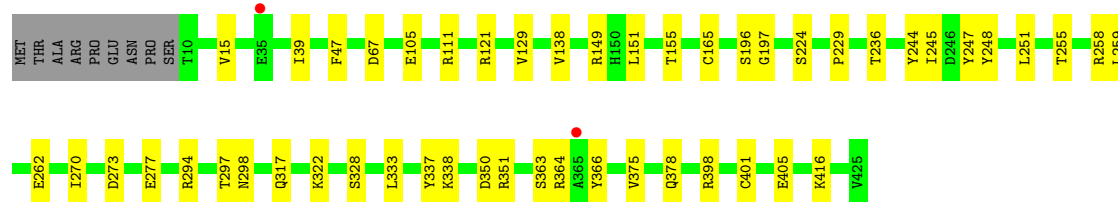
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	G	1	Total 53	C 27	N 9	O 15	P 2	0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

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Monooxygenase

Chain A:  86% 12% .




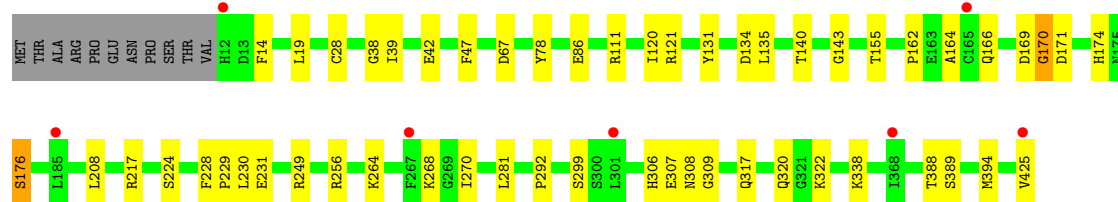
#### • Molecule 1: Monooxygenase

Chain B:  83% 15% .




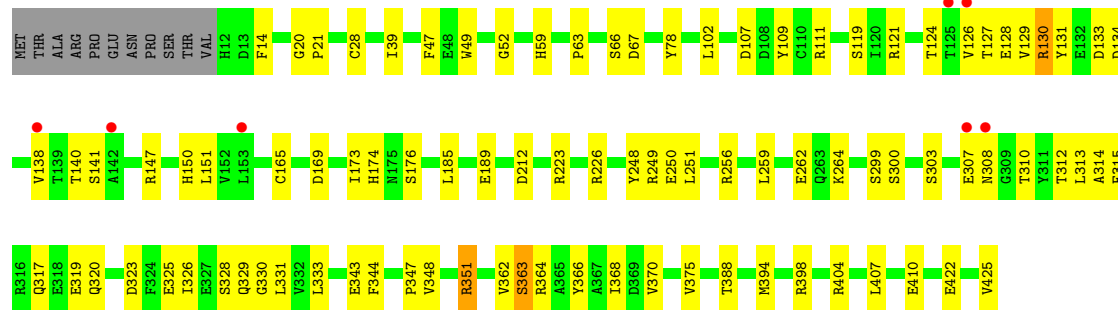
#### • Molecule 1: Monooxygenase

Chain C:  85% 12% .




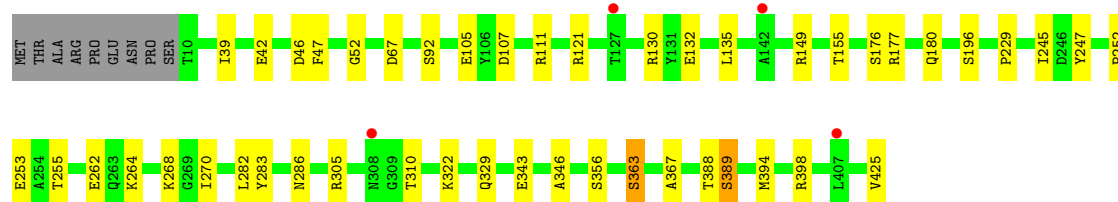
#### • Molecule 1: Monooxygenase

Chain D:  76% 21% 2%




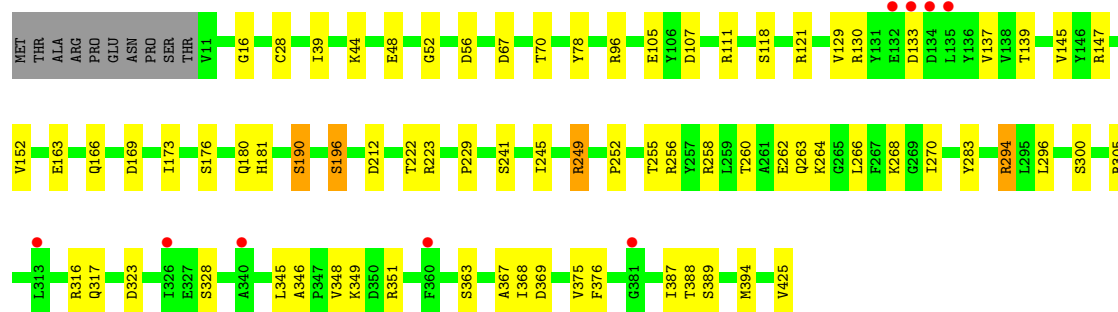
• Molecule 1: Monooxygenase

Chain E:  87% 11% 2%




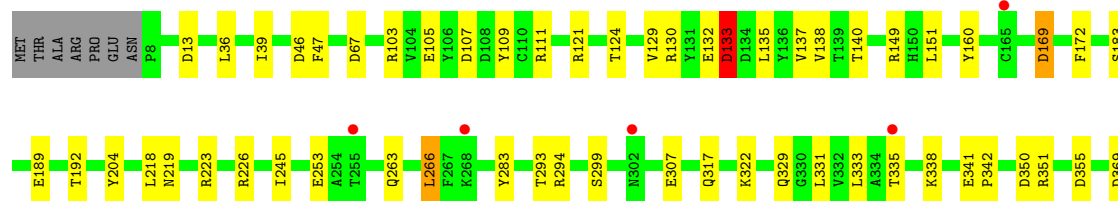
• Molecule 1: Monooxygenase

Chain F:  80% 17% 2%



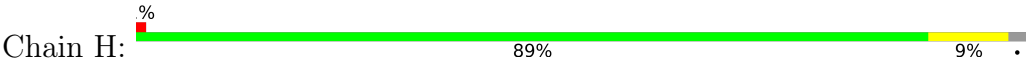
• Molecule 1: Monooxygenase

Chain G:  83% 14% 2%





● Molecule 1: Monooxygenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.05Å 151.17Å 141.40Å 90.00° 91.58° 90.00°	Depositor
Resolution (Å)	39.12 – 2.86 47.47 – 2.86	Depositor EDS
% Data completeness (in resolution range)	91.6 (39.12-2.86) 91.7 (47.47-2.86)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.199 , 0.258 0.200 , 0.258	Depositor DCC
$R_{free}$ test set	3619 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 28.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	27122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3296e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/3425	0.45	0/4653
1	B	0.27	0/3425	0.46	2/4653 (0.0%)
1	C	0.27	0/3411	0.44	0/4633
1	D	0.27	0/3411	0.48	1/4633 (0.0%)
1	E	0.27	0/3425	0.44	0/4653
1	F	0.26	0/3418	0.44	0/4643
1	G	0.30	0/3439	0.45	0/4672
1	H	0.27	0/3425	0.43	0/4653
All	All	0.27	0/27379	0.45	3/37193 (0.0%)

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	D	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	D	133	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	217	ARG	NE-CZ-NH2	5.34	122.97	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	169	ASP	Peptide
1	G	133	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	3340	0	3221	32	0
1	B	3340	0	3221	39	0
1	C	3326	0	3205	40	0
1	D	3326	0	3205	63	0
1	E	3340	0	3221	29	0
1	F	3333	0	3214	44	0
1	G	3353	0	3234	37	0
1	H	3340	0	3221	23	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	0	0
2	G	53	0	31	2	0
2	H	53	0	31	2	0
All	All	27122	0	25990	291	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 5.

All (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:O	1:A:338:LYS:HD2	1.51	1.08
1:E:343:GLU:OE2	1:E:343:GLU:O	1.82	0.98
1:C:317:GLN:OE1	1:C:320:GLN:HB3	1.69	0.92
1:D:317:GLN:OE1	1:D:320:GLN:N	2.06	0.88
1:G:151:LEU:HB2	1:G:375:VAL:HG12	1.58	0.85
1:F:294:ARG:HH21	1:F:296:LEU:HD11	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:GLN:OE1	1:C:320:GLN:CB	2.26	0.83
1:B:313:LEU:HD11	1:B:331:LEU:HD13	1.60	0.81
1:F:96:ARG:O	1:H:234:LYS:NZ	2.18	0.76
1:B:294:ARG:HE	1:B:296:LEU:HD11	1.52	0.74
1:D:317:GLN:CD	1:D:320:GLN:H	1.92	0.73
1:G:129:VAL:HG22	1:G:138:VAL:HG12	1.71	0.72
1:A:151:LEU:HB2	1:A:375:VAL:HG13	1.73	0.71
1:D:313:LEU:HD12	1:D:326:ILE:HD11	1.74	0.69
1:E:388:THR:HB	1:E:394:MET:HG3	1.74	0.69
1:F:163:GLU:HA	1:F:166:GLN:HG2	1.73	0.69
1:C:317:GLN:HE22	1:C:320:GLN:HB2	1.56	0.68
1:D:174:HIS:ND1	1:D:176:SER:OG	2.24	0.68
1:G:172:PHE:HB2	1:G:331:LEU:HD12	1.75	0.68
1:C:317:GLN:NE2	1:C:320:GLN:H	1.92	0.68
1:D:131:TYR:CZ	1:D:134:ASP:HA	2.28	0.68
1:F:425:VAL:HG23	1:G:322:LYS:HD2	1.76	0.67
1:A:39:ILE:HD11	1:A:121:ARG:HH11	1.60	0.66
1:G:350:ASP:OD1	1:G:351:ARG:N	2.30	0.64
1:B:304:ALA:CB	1:B:313:LEU:HD23	2.28	0.63
1:A:378:GLN:OE1	1:A:398:ARG:NH1	2.32	0.63
1:F:363:SER:HB3	1:F:367:ALA:H	1.63	0.63
1:C:140:THR:OG1	1:C:143:GLY:N	2.31	0.63
1:D:130:ARG:HB3	1:D:347:PRO:HB2	1.80	0.62
1:G:13:ASP:OD1	1:G:149:ARG:NH1	2.32	0.62
1:E:130:ARG:NH1	1:E:132:GLU:OE2	2.28	0.62
1:C:42:GLU:OE2	2:C:501:FAD:H1B	1.98	0.62
1:F:52:GLY:HA2	1:F:180:GLN:HE22	1.65	0.62
1:A:247:TYR:O	1:A:251:LEU:HD13	2.00	0.61
1:F:241:SER:O	1:F:245:ILE:HG13	2.00	0.61
1:B:129:VAL:HG22	1:B:138:VAL:HG12	1.83	0.61
1:D:128:GLU:HA	1:D:344:PHE:HB2	1.82	0.61
1:C:317:GLN:NE2	1:C:320:GLN:HB2	2.14	0.60
1:G:107:ASP:OD2	1:G:111:ARG:NH2	2.34	0.60
1:D:28:CYS:HB3	1:D:78:TYR:HD2	1.64	0.60
1:B:253:GLU:OE2	1:B:356:SER:OG	2.19	0.60
1:A:255:THR:HG22	1:A:258:ARG:HH22	1.66	0.60
1:D:107:ASP:OD1	1:D:111:ARG:NH2	2.33	0.60
1:D:317:GLN:OE1	1:D:317:GLN:C	2.39	0.60
1:G:189:GLU:HB2	1:G:329:GLN:OE1	2.01	0.60
1:B:140:THR:HG22	1:B:142:ALA:H	1.65	0.60
1:C:217:ARG:HG3	1:C:292:PRO:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:HD22	1:B:387:ILE:HG22	1.84	0.59
1:D:303:SER:HB2	1:D:314:ALA:HB3	1.85	0.59
1:D:404:ARG:HG3	1:D:410:GLU:HG3	1.83	0.59
1:C:317:GLN:OE1	1:C:320:GLN:HB2	2.03	0.59
1:F:263:GLN:HG2	1:F:266:LEU:HB2	1.85	0.59
1:F:369:ASP:HB3	1:F:375:VAL:HG12	1.83	0.58
1:D:249:ARG:O	1:D:256:ARG:NH1	2.37	0.58
1:D:129:VAL:HG22	1:D:138:VAL:HG12	1.86	0.58
1:F:258:ARG:O	1:F:262:GLU:HG3	2.04	0.57
1:H:392:LEU:N	2:H:501:FAD:O2	2.32	0.57
1:H:107:ASP:OD2	1:H:111:ARG:NH1	2.38	0.57
1:F:129:VAL:HG11	1:F:345:LEU:HD23	1.87	0.57
1:B:31:GLU:HG3	1:B:117:LEU:HD22	1.86	0.57
1:C:39:ILE:HD11	1:C:121:ARG:NE	2.20	0.56
1:D:249:ARG:HH11	1:D:249:ARG:HG3	1.70	0.56
1:F:107:ASP:OD2	1:F:111:ARG:NH2	2.34	0.56
1:D:259:LEU:HA	1:D:262:GLU:HG2	1.88	0.56
1:D:368:ILE:HG13	1:D:375:VAL:HG13	1.87	0.56
1:D:49:TRP:NE1	2:D:501:FAD:O4'	2.36	0.56
1:F:348:VAL:HG12	1:F:351:ARG:HB2	1.88	0.56
1:A:351:ARG:HG2	1:A:351:ARG:HH11	1.70	0.55
1:E:245:ILE:HD11	1:E:388:THR:HG21	1.89	0.55
1:B:304:ALA:HB1	1:B:313:LEU:HD23	1.88	0.55
1:C:47:PHE:HB3	1:C:111:ARG:HG2	1.88	0.55
1:B:190:SER:HB2	1:B:329:GLN:H	1.72	0.55
1:F:44:LYS:HD3	1:F:48:GLU:HG2	1.88	0.54
1:B:56:ASP:N	1:B:56:ASP:OD1	2.39	0.54
1:F:130:ARG:HG3	1:F:137:VAL:HG23	1.89	0.54
1:E:322:LYS:HD3	1:H:425:VAL:HG23	1.90	0.54
1:G:39:ILE:HD11	1:G:121:ARG:HE	1.72	0.54
1:D:28:CYS:HB3	1:D:78:TYR:CD2	2.42	0.54
1:C:317:GLN:NE2	1:C:320:GLN:N	2.56	0.53
1:G:218:LEU:HB3	1:G:293:THR:HG23	1.91	0.53
1:D:388:THR:HB	1:D:394:MET:HG3	1.90	0.53
1:H:241:SER:HB2	1:H:418:ILE:HG12	1.89	0.53
1:B:260:THR:HG21	1:B:383:HIS:HA	1.91	0.53
1:B:107:ASP:OD2	1:B:111:ARG:NH2	2.39	0.53
1:C:388:THR:HB	1:C:394:MET:HG3	1.91	0.53
1:G:124:THR:HG23	1:G:140:THR:HG23	1.90	0.53
1:D:127:THR:O	1:D:128:GLU:HG3	2.09	0.53
1:D:223:ARG:HA	1:D:299:SER:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ARG:HH21	1:C:256:ARG:HH22	1.56	0.53
1:F:28:CYS:HB3	1:F:78:TYR:CD2	2.44	0.52
1:C:308:ASN:CG	1:C:309:GLY:H	2.13	0.52
1:A:255:THR:HG22	1:A:258:ARG:NH2	2.25	0.52
1:E:363:SER:HB3	1:E:367:ALA:H	1.75	0.52
1:B:322:LYS:HD3	1:C:425:VAL:HG23	1.90	0.52
1:G:105:GLU:OE2	1:H:283:TYR:OH	2.17	0.52
1:H:212:ASP:OD1	1:H:285:LYS:NZ	2.37	0.52
1:F:139:THR:HB	1:F:145:VAL:HG23	1.92	0.51
1:A:105:GLU:OE2	1:B:283:TYR:OH	2.18	0.51
1:A:224:SER:O	1:A:297:THR:OG1	2.26	0.51
1:E:252:PRO:HB2	1:E:255:THR:HG23	1.92	0.51
1:F:368:ILE:HG13	1:F:375:VAL:HG13	1.93	0.51
1:A:15:VAL:HG12	1:A:39:ILE:HG22	1.91	0.51
1:A:129:VAL:HG22	1:A:138:VAL:HG12	1.92	0.51
1:B:194:VAL:HB	1:B:333:LEU:HD13	1.92	0.50
1:A:322:LYS:HD3	1:D:425:VAL:HG13	1.93	0.50
1:B:400:SER:HB3	1:B:414:VAL:HG22	1.94	0.50
1:H:83:TYR:O	1:H:87:LYS:HG2	2.11	0.50
1:E:196:SER:HB3	1:E:268:LYS:HD2	1.93	0.50
1:F:388:THR:HB	1:F:394:MET:HG3	1.92	0.50
1:H:241:SER:O	1:H:245:ILE:HG13	2.11	0.50
1:E:343:GLU:CD	1:E:346:ALA:HB2	2.32	0.50
1:B:346:ALA:HA	1:B:349:LYS:HG3	1.94	0.50
1:F:16:GLY:HA2	1:F:152:VAL:HG23	1.93	0.50
1:D:63:PRO:O	1:D:66:SER:OG	2.29	0.49
1:D:315:PHE:HE2	1:D:326:ILE:HG12	1.77	0.49
1:D:126:VAL:HG22	2:D:501:FAD:N1A	2.27	0.49
1:C:299:SER:HA	1:C:317:GLN:HA	1.94	0.49
1:D:364:ARG:O	1:D:364:ARG:NH1	2.42	0.49
1:G:133:ASP:HB2	1:G:135:LEU:HG	1.93	0.49
1:G:392:LEU:HG	2:G:501:FAD:C2	2.42	0.49
1:F:212:ASP:OD1	1:F:212:ASP:N	2.39	0.49
1:A:350:ASP:OD1	1:A:350:ASP:N	2.45	0.49
1:A:401:CYS:O	1:A:405:GLU:HG2	2.13	0.49
1:E:343:GLU:OE1	1:E:346:ALA:HB2	2.13	0.49
1:C:28:CYS:HB3	1:C:78:TYR:CD2	2.47	0.49
1:C:131:TYR:CZ	1:C:134:ASP:HA	2.47	0.49
1:D:314:ALA:HA	1:D:325:GLU:HG2	1.94	0.49
1:F:266:LEU:HD22	1:F:387:ILE:HG22	1.93	0.49
1:B:245:ILE:HD11	1:B:388:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:OG1	1:D:226:ARG:NH1	2.46	0.49
1:D:119:SER:OG	1:D:119:SER:O	2.30	0.49
1:E:389:SER:HA	1:E:398:ARG:HH12	1.77	0.49
1:D:328:SER:OG	1:D:330:GLY:O	2.31	0.49
1:B:223:ARG:HE	1:B:300:SER:HB2	1.78	0.48
1:E:283:TYR:OH	1:F:105:GLU:OE2	2.22	0.48
1:C:264:LYS:NZ	1:C:268:LYS:HD3	2.28	0.48
1:D:39:ILE:HD12	1:D:121:ARG:NH2	2.28	0.48
1:F:262:GLU:O	1:F:264:LYS:HG3	2.13	0.48
1:D:150:HIS:O	1:D:151:LEU:HD23	2.14	0.48
1:H:89:ARG:NH1	1:H:105:GLU:OE2	2.47	0.48
1:A:258:ARG:O	1:A:262:GLU:HG3	2.13	0.48
1:A:229:PRO:HA	1:A:270:ILE:O	2.14	0.48
1:E:343:GLU:OE2	1:E:343:GLU:C	2.49	0.48
1:A:294:ARG:NH1	1:D:422:GLU:OE1	2.47	0.47
1:B:232:TYR:HA	1:B:237:LEU:HD21	1.96	0.47
1:C:171:ASP:N	1:C:171:ASP:OD1	2.47	0.47
1:D:300:SER:O	1:D:315:PHE:HD1	1.97	0.47
1:G:103:ARG:NH1	2:G:501:FAD:H6	2.27	0.47
1:A:366:TYR:CD1	1:A:398:ARG:HD3	2.49	0.47
1:D:52:GLY:HA3	1:D:176:SER:O	2.14	0.47
1:D:404:ARG:NH1	1:D:410:GLU:OE1	2.48	0.47
1:F:249:ARG:HH21	1:F:256:ARG:NH2	2.12	0.47
1:C:224:SER:HB3	1:C:228:PHE:HE2	1.80	0.47
1:G:253:GLU:OE2	1:G:355:ASP:HB2	2.14	0.47
1:D:124:THR:HG23	1:D:140:THR:CG2	2.45	0.47
1:D:249:ARG:NH2	1:D:363:SER:HA	2.29	0.47
1:D:366:TYR:CE1	1:D:398:ARG:HG3	2.50	0.47
1:F:348:VAL:HG12	1:F:348:VAL:O	2.14	0.47
1:C:155:THR:O	2:C:501:FAD:H51A	2.14	0.47
1:H:186:VAL:HG13	1:H:216:TYR:HE2	1.80	0.47
1:A:245:ILE:HG13	1:A:364:ARG:HE	1.79	0.47
1:A:364:ARG:HG3	1:A:364:ARG:HH11	1.80	0.47
1:E:253:GLU:OE2	1:E:356:SER:OG	2.31	0.46
1:C:19:LEU:HD22	1:C:120:ILE:HG21	1.97	0.46
1:F:173:ILE:HD13	1:F:181:HIS:HB2	1.97	0.46
1:E:247:TYR:OH	1:H:319:GLU:OE1	2.20	0.46
1:F:52:GLY:HA2	1:F:180:GLN:NE2	2.30	0.46
1:G:223:ARG:HA	1:G:299:SER:H	1.80	0.46
1:B:163:GLU:HA	1:B:166:GLN:HG3	1.96	0.46
1:F:256:ARG:O	1:F:260:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:LEU:HB3	1:G:335:THR:HG23	1.97	0.46
1:B:425:VAL:HG23	1:C:322:LYS:HD3	1.98	0.46
1:D:173:ILE:HD11	1:D:185:LEU:HD11	1.98	0.46
1:F:316:ARG:HG3	1:F:323:ASP:OD1	2.16	0.46
1:E:310:THR:HG22	1:E:329:GLN:HG2	1.97	0.46
1:F:52:GLY:HA3	1:F:176:SER:O	2.15	0.46
1:A:196:SER:OG	1:A:197:GLY:N	2.49	0.45
1:C:208:LEU:HG	1:C:281:LEU:HD23	1.97	0.45
1:C:317:GLN:CD	1:C:320:GLN:CB	2.84	0.45
1:E:105:GLU:OE2	1:F:283:TYR:OH	2.24	0.45
1:A:47:PHE:HB3	1:A:111:ARG:HG2	1.99	0.45
1:A:15:VAL:HG12	1:A:39:ILE:CG2	2.47	0.45
1:C:224:SER:OG	1:C:264:LYS:NZ	2.48	0.45
1:F:196:SER:HB2	1:F:222:THR:OG1	2.16	0.45
1:C:317:GLN:CD	1:C:320:GLN:HB2	2.37	0.45
1:E:42:GLU:OE1	2:E:501:FAD:H1B	2.16	0.45
1:F:67:ASP:CG	1:F:70:THR:HG1	2.20	0.45
1:A:273:ASP:O	1:A:277:GLU:HG2	2.17	0.45
1:D:351:ARG:O	1:D:370:VAL:HG13	2.17	0.45
1:B:304:ALA:HB2	1:B:313:LEU:HD23	1.99	0.45
1:D:317:GLN:OE1	1:D:317:GLN:O	2.35	0.44
1:B:168:LEU:HD22	1:B:311:TYR:HE1	1.81	0.44
1:F:369:ASP:HB3	1:F:375:VAL:CG1	2.46	0.44
1:G:192:THR:HG23	1:G:219:ASN:HB2	1.99	0.44
1:D:165:CYS:SG	1:D:333:LEU:HD21	2.57	0.44
1:B:15:VAL:HG22	1:B:39:ILE:HG22	1.99	0.44
1:C:162:PRO:O	1:C:164:ALA:N	2.41	0.44
1:C:174:HIS:ND1	1:C:176:SER:HB2	2.32	0.44
1:D:307:GLU:HG2	1:D:310:THR:HG23	2.00	0.44
1:A:155:THR:C	2:A:501:FAD:H52A	2.38	0.44
1:F:252:PRO:O	1:F:255:THR:OG1	2.27	0.44
1:C:134:ASP:O	1:C:135:LEU:HD23	2.17	0.44
1:C:338:LYS:HE3	1:C:338:LYS:HB3	1.87	0.44
1:E:282:LEU:O	1:E:286:ASN:HB2	2.17	0.44
1:B:39:ILE:HD11	1:B:121:ARG:CZ	2.48	0.44
1:D:39:ILE:HA	1:D:119:SER:OG	2.17	0.43
1:F:39:ILE:HD11	1:F:121:ARG:NE	2.32	0.43
1:C:170:GLY:H	1:C:306:HIS:CD2	2.37	0.43
1:D:131:TYR:OH	1:D:134:ASP:HA	2.18	0.43
1:D:14:PHE:HA	1:D:150:HIS:O	2.19	0.43
1:E:229:PRO:HA	1:E:270:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:PRO:HA	1:H:270:ILE:O	2.18	0.43
1:C:140:THR:HG1	1:C:143:GLY:H	1.62	0.43
1:C:249:ARG:O	1:C:256:ARG:NH1	2.51	0.43
1:E:425:VAL:HB	1:H:322:LYS:HD3	2.00	0.43
1:F:229:PRO:HA	1:F:270:ILE:O	2.19	0.43
1:G:36:LEU:HD23	1:G:36:LEU:HA	1.83	0.43
1:G:369:ASP:HB3	1:G:375:VAL:HG22	2.01	0.43
1:C:229:PRO:HG2	1:C:231:GLU:HG3	2.01	0.43
1:B:149:ARG:HB2	1:B:150:HIS:CD2	2.54	0.42
1:E:135:LEU:CD2	1:E:149:ARG:HG3	2.49	0.42
1:G:39:ILE:HD11	1:G:121:ARG:NE	2.34	0.42
1:D:248:TYR:HA	1:D:251:LEU:HD13	1.99	0.42
1:G:130:ARG:HE	1:G:130:ARG:HB2	1.58	0.42
1:G:263:GLN:HG2	1:G:266:LEU:HB2	2.01	0.42
1:A:245:ILE:HG13	1:A:364:ARG:NE	2.34	0.42
1:D:317:GLN:HE22	1:D:319:GLU:HB3	1.84	0.42
1:D:343:GLU:H	1:D:343:GLU:CD	2.22	0.42
1:D:362:VAL:HG12	1:D:366:TYR:HA	2.00	0.42
1:H:256:ARG:O	1:H:260:THR:HG23	2.19	0.42
1:H:182:ARG:O	1:H:186:VAL:HG23	2.19	0.42
1:B:247:TYR:CZ	1:B:251:LEU:HD11	2.55	0.42
1:F:223:ARG:HG3	1:F:300:SER:HB2	2.02	0.42
1:G:46:ASP:OD1	1:G:47:PHE:N	2.50	0.42
1:H:52:GLY:HA3	1:H:176:SER:O	2.19	0.42
1:G:160:TYR:CD1	1:G:338:LYS:HD2	2.55	0.42
1:E:177:ARG:HD2	1:E:180:GLN:OE1	2.18	0.42
1:G:169:ASP:OD1	1:G:169:ASP:N	2.52	0.42
1:G:404:ARG:HD3	1:G:410:GLU:HG3	2.02	0.42
1:D:313:LEU:HD11	1:D:331:LEU:HD13	2.02	0.42
1:H:364:ARG:NH2	1:H:397:TYR:OH	2.50	0.42
1:D:59:HIS:HA	1:D:102:LEU:HA	2.02	0.42
1:F:152:VAL:HG12	1:F:376:PHE:HB2	2.02	0.42
1:B:144:ASP:OD1	1:B:144:ASP:N	2.53	0.41
1:F:190:SER:OG	1:F:328:SER:HA	2.20	0.41
1:G:132:GLU:HB2	1:G:137:VAL:HG21	2.02	0.41
1:A:165:CYS:SG	1:A:333:LEU:HD11	2.60	0.41
1:B:131:TYR:CZ	1:B:134:ASP:HA	2.55	0.41
1:C:249:ARG:HH21	1:C:256:ARG:HH12	1.67	0.41
1:D:189:GLU:H	1:D:329:GLN:NE2	2.17	0.41
1:E:46:ASP:OD1	1:E:47:PHE:N	2.52	0.41
1:H:50:HIS:CG	2:H:501:FAD:HM82	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:GLN:NE2	1:G:226:ARG:HH22	2.17	0.41
1:A:297:THR:OG1	1:A:298:ASN:N	2.53	0.41
1:B:253:GLU:OE2	1:B:355:ASP:HB2	2.21	0.41
1:B:304:ALA:CB	1:B:313:LEU:CD2	2.97	0.41
1:D:20:GLY:HA3	1:D:47:PHE:HE2	1.86	0.41
1:E:107:ASP:OD2	1:E:111:ARG:NH2	2.41	0.41
1:E:305:ARG:HE	1:E:305:ARG:HB3	1.71	0.41
1:C:14:PHE:CZ	1:C:38:GLY:HA3	2.55	0.41
1:D:140:THR:HG22	1:D:141:SER:N	2.35	0.41
1:G:350:ASP:OD1	1:G:351:ARG:HG3	2.21	0.41
1:G:404:ARG:HH12	1:G:416:LYS:NZ	2.18	0.41
1:B:118:SER:O	1:B:118:SER:OG	2.38	0.41
1:B:128:GLU:OE2	1:B:130:ARG:HD3	2.21	0.41
1:D:348:VAL:HG22	1:D:351:ARG:HB2	2.02	0.41
1:C:229:PRO:HA	1:C:270:ILE:O	2.21	0.41
1:D:124:THR:HG23	1:D:140:THR:HG23	2.02	0.41
1:D:212:ASP:OD1	1:D:212:ASP:N	2.49	0.41
1:D:310:THR:HA	1:D:329:GLN:HA	2.03	0.41
1:F:16:GLY:N	1:F:39:ILE:O	2.44	0.41
1:G:283:TYR:HD2	1:H:92:SER:HG	1.69	0.41
1:G:341:GLU:HA	1:G:342:PRO:HD3	1.90	0.41
1:B:50:HIS:CG	2:B:501:FAD:HM82	2.56	0.41
1:E:52:GLY:HA3	1:E:176:SER:O	2.21	0.41
1:B:52:GLY:HA3	1:B:176:SER:O	2.21	0.40
1:E:155:THR:C	2:E:501:FAD:H52A	2.42	0.40
1:F:346:ALA:HA	1:F:349:LYS:HG3	2.02	0.40
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.83	0.40
1:B:229:PRO:HA	1:B:270:ILE:O	2.21	0.40
1:G:245:ILE:HD11	1:G:388:THR:HG21	2.04	0.40
1:H:46:ASP:OD1	1:H:47:PHE:N	2.54	0.40
1:H:235:LEU:HA	1:H:235:LEU:HD23	1.85	0.40
1:G:36:LEU:HG	1:G:407:LEU:HD13	2.03	0.40
1:H:305:ARG:HE	1:H:305:ARG:HB2	1.75	0.40
1:A:244:TYR:O	1:A:248:TYR:N	2.43	0.40
1:B:404:ARG:HD3	1:B:410:GLU:HG2	2.03	0.40
1:D:21:PRO:HD2	2:D:501:FAD:O5'	2.21	0.40
1:D:307:GLU:OE2	1:D:312:THR:OG1	2.39	0.40
1:E:39:ILE:HD11	1:E:121:ARG:NE	2.36	0.40
1:G:204:TYR:OH	1:G:293:THR:HG21	2.21	0.40

There are no symmetry-related clashes.

## 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	414/425 (97%)	391 (94%)	22 (5%)	1 (0%)	47	75
1	B	414/425 (97%)	391 (94%)	22 (5%)	1 (0%)	47	75
1	C	412/425 (97%)	387 (94%)	21 (5%)	4 (1%)	15	40
1	D	412/425 (97%)	392 (95%)	18 (4%)	2 (0%)	29	57
1	E	414/425 (97%)	393 (95%)	20 (5%)	1 (0%)	47	75
1	F	413/425 (97%)	395 (96%)	18 (4%)	0	100	100
1	G	416/425 (98%)	392 (94%)	21 (5%)	3 (1%)	22	50
1	H	414/425 (97%)	393 (95%)	20 (5%)	1 (0%)	47	75
All	All	3309/3400 (97%)	3134 (95%)	162 (5%)	13 (0%)	34	62

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	170	GLY
1	D	67	ASP
1	D	308	ASN
1	G	266	LEU
1	A	67	ASP
1	C	67	ASP
1	C	169	ASP
1	B	67	ASP
1	G	67	ASP
1	G	307	GLU
1	C	230	LEU
1	E	67	ASP
1	H	67	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/367 (98%)	354 (99%)	5 (1%)	67	86
1	B	359/367 (98%)	356 (99%)	3 (1%)	81	93
1	C	357/367 (97%)	352 (99%)	5 (1%)	67	86
1	D	357/367 (97%)	348 (98%)	9 (2%)	47	76
1	E	359/367 (98%)	354 (99%)	5 (1%)	67	86
1	F	358/367 (98%)	345 (96%)	13 (4%)	35	66
1	G	361/367 (98%)	354 (98%)	7 (2%)	57	81
1	H	359/367 (98%)	354 (99%)	5 (1%)	67	86
All	All	2869/2936 (98%)	2817 (98%)	52 (2%)	59	82

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ARG
1	A	317	GLN
1	A	328	SER
1	A	363	SER
1	A	416	LYS
1	B	144	ASP
1	B	237	LEU
1	B	377	LEU
1	C	86	GLU
1	C	166	GLN
1	C	176	SER
1	C	307	GLU
1	C	389	SER
1	D	109	TYR
1	D	130	ARG
1	D	147	ARG
1	D	250	GLU
1	D	264	LYS
1	D	323	ASP

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Mol	Chain	Res	Type
1	D	351	ARG
1	D	363	SER
1	D	407	LEU
1	E	92	SER
1	E	262	GLU
1	E	264	LYS
1	E	363	SER
1	E	389	SER
1	F	56	ASP
1	F	118	SER
1	F	133	ASP
1	F	147	ARG
1	F	169	ASP
1	F	190	SER
1	F	196	SER
1	F	249	ARG
1	F	268	LYS
1	F	294	ARG
1	F	305	ARG
1	F	317	GLN
1	F	389	SER
1	G	109	TYR
1	G	133	ASP
1	G	169	ASP
1	G	183	SER
1	G	294	ARG
1	G	317	GLN
1	G	389	SER
1	H	133	ASP
1	H	212	ASP
1	H	317	GLN
1	H	389	SER
1	H	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	A	357	GLN
1	B	263	GLN
1	C	306	HIS
1	D	166	GLN

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Mol	Chain	Res	Type
1	D	329	GLN
1	D	357	GLN
1	F	180	GLN
1	G	180	GLN
1	G	329	GLN
1	H	115	ASN

### 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	D	501	-	51,58,58	1.22	5 (9%)	60,89,89	2.20	7 (11%)
2	FAD	E	501	-	51,58,58	1.21	6 (11%)	60,89,89	2.21	7 (11%)
2	FAD	B	501	-	51,58,58	1.22	5 (9%)	60,89,89	2.21	7 (11%)
2	FAD	F	501	-	51,58,58	1.22	5 (9%)	60,89,89	2.21	7 (11%)
2	FAD	H	501	-	51,58,58	1.21	5 (9%)	60,89,89	2.22	7 (11%)
2	FAD	G	501	-	51,58,58	1.21	5 (9%)	60,89,89	2.21	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	A	501	-	51,58,58	1.22	5 (9%)	60,89,89	2.22	7 (11%)
2	FAD	C	501	-	51,58,58	1.22	5 (9%)	60,89,89	2.22	7 (11%)

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	D	501	-	-	5/30/50/50	0/6/6/6
2	FAD	E	501	-	-	5/30/50/50	0/6/6/6
2	FAD	B	501	-	-	9/30/50/50	0/6/6/6
2	FAD	F	501	-	-	3/30/50/50	0/6/6/6
2	FAD	H	501	-	-	5/30/50/50	0/6/6/6
2	FAD	G	501	-	-	10/30/50/50	0/6/6/6
2	FAD	A	501	-	-	6/30/50/50	0/6/6/6
2	FAD	C	501	-	-	14/30/50/50	0/6/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C4X-C10	5.72	1.44	1.38
2	G	501	FAD	C4X-C10	5.72	1.44	1.38
2	D	501	FAD	C4X-C10	5.70	1.44	1.38
2	C	501	FAD	C4X-C10	5.70	1.44	1.38
2	B	501	FAD	C4X-C10	5.69	1.44	1.38
2	E	501	FAD	C4X-C10	5.64	1.44	1.38
2	H	501	FAD	C4X-C10	5.64	1.44	1.38
2	F	501	FAD	C4X-C10	5.61	1.44	1.38
2	B	501	FAD	C4-N3	3.17	1.38	1.33
2	F	501	FAD	C4-N3	3.14	1.38	1.33
2	C	501	FAD	C4-N3	3.08	1.38	1.33
2	D	501	FAD	C4-N3	3.01	1.38	1.33
2	A	501	FAD	C4-N3	2.96	1.38	1.33
2	E	501	FAD	C4-N3	2.94	1.38	1.33
2	H	501	FAD	C4-N3	2.87	1.38	1.33
2	G	501	FAD	C4-N3	2.85	1.38	1.33
2	D	501	FAD	C4-C4X	2.54	1.45	1.41
2	B	501	FAD	C4-C4X	2.48	1.45	1.41
2	F	501	FAD	C4-C4X	2.45	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C4-C4X	2.43	1.45	1.41
2	C	501	FAD	C4-C4X	2.42	1.45	1.41
2	E	501	FAD	C4-C4X	2.41	1.45	1.41
2	G	501	FAD	C4-C4X	2.39	1.45	1.41
2	H	501	FAD	C4-C4X	2.38	1.45	1.41
2	B	501	FAD	C9A-N10	2.35	1.41	1.38
2	F	501	FAD	C9A-N10	2.35	1.41	1.38
2	H	501	FAD	C9A-N10	2.34	1.41	1.38
2	E	501	FAD	C9A-N10	2.31	1.41	1.38
2	D	501	FAD	C5X-N5	2.31	1.39	1.35
2	D	501	FAD	C9A-N10	2.28	1.41	1.38
2	A	501	FAD	C5X-N5	2.27	1.39	1.35
2	A	501	FAD	C9A-N10	2.27	1.41	1.38
2	E	501	FAD	C5X-N5	2.25	1.39	1.35
2	B	501	FAD	C5X-N5	2.23	1.39	1.35
2	G	501	FAD	C9A-N10	2.23	1.41	1.38
2	F	501	FAD	C5X-N5	2.22	1.39	1.35
2	C	501	FAD	C5X-N5	2.21	1.39	1.35
2	C	501	FAD	C9A-N10	2.20	1.41	1.38
2	G	501	FAD	C5X-N5	2.18	1.38	1.35
2	H	501	FAD	C5X-N5	2.09	1.38	1.35
2	E	501	FAD	C4X-N5	-2.04	1.30	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C4-N3-C2	13.01	126.13	115.14
2	C	501	FAD	C4-N3-C2	13.01	126.12	115.14
2	G	501	FAD	C4-N3-C2	12.99	126.11	115.14
2	B	501	FAD	C4-N3-C2	12.98	126.10	115.14
2	H	501	FAD	C4-N3-C2	12.96	126.09	115.14
2	D	501	FAD	C4-N3-C2	12.96	126.08	115.14
2	F	501	FAD	C4-N3-C2	12.95	126.08	115.14
2	E	501	FAD	C4-N3-C2	12.91	126.04	115.14
2	D	501	FAD	C4X-C4-N3	-7.06	113.78	123.43
2	B	501	FAD	C4X-C4-N3	-7.03	113.82	123.43
2	C	501	FAD	C4X-C4-N3	-7.01	113.84	123.43
2	H	501	FAD	C4X-C4-N3	-7.00	113.86	123.43
2	G	501	FAD	C4X-C4-N3	-6.99	113.86	123.43
2	A	501	FAD	C4X-C4-N3	-6.99	113.87	123.43
2	E	501	FAD	C4X-C4-N3	-6.99	113.87	123.43
2	F	501	FAD	C4X-C4-N3	-6.95	113.93	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C10-C4X-N5	4.79	124.57	121.26
2	E	501	FAD	C10-C4X-N5	4.78	124.57	121.26
2	H	501	FAD	C10-C4X-N5	4.74	124.54	121.26
2	F	501	FAD	C10-C4X-N5	4.74	124.53	121.26
2	B	501	FAD	C10-C4X-N5	4.72	124.52	121.26
2	G	501	FAD	C10-C4X-N5	4.68	124.50	121.26
2	C	501	FAD	C10-C4X-N5	4.66	124.48	121.26
2	D	501	FAD	C10-C4X-N5	4.54	124.39	121.26
2	H	501	FAD	C4-C4X-C10	-3.75	117.47	119.95
2	B	501	FAD	C4-C4X-C10	-3.73	117.48	119.95
2	F	501	FAD	C4-C4X-C10	-3.70	117.50	119.95
2	E	501	FAD	C4-C4X-C10	-3.69	117.51	119.95
2	C	501	FAD	C4-C4X-C10	-3.69	117.51	119.95
2	D	501	FAD	C4-C4X-C10	-3.68	117.51	119.95
2	A	501	FAD	C4-C4X-C10	-3.68	117.52	119.95
2	G	501	FAD	C4-C4X-C10	-3.60	117.57	119.95
2	A	501	FAD	C4X-C10-N10	-3.54	116.67	120.30
2	H	501	FAD	C4X-C10-N10	-3.50	116.71	120.30
2	F	501	FAD	C4X-C10-N10	-3.48	116.72	120.30
2	B	501	FAD	C4X-C10-N10	-3.48	116.72	120.30
2	E	501	FAD	C4X-C10-N10	-3.44	116.76	120.30
2	C	501	FAD	C4X-C10-N10	-3.43	116.78	120.30
2	G	501	FAD	C4X-C10-N10	-3.43	116.78	120.30
2	D	501	FAD	C4X-C10-N10	-3.42	116.79	120.30
2	H	501	FAD	C1'-N10-C9A	3.08	120.72	118.29
2	G	501	FAD	C1'-N10-C9A	3.02	120.67	118.29
2	E	501	FAD	C1'-N10-C9A	3.02	120.67	118.29
2	F	501	FAD	C1'-N10-C9A	3.01	120.66	118.29
2	B	501	FAD	C1'-N10-C9A	2.97	120.63	118.29
2	C	501	FAD	C1'-N10-C9A	2.93	120.60	118.29
2	D	501	FAD	C1'-N10-C9A	2.88	120.56	118.29
2	A	501	FAD	C1'-N10-C9A	2.88	120.56	118.29
2	H	501	FAD	C5A-C6A-N6A	2.31	123.87	120.35
2	F	501	FAD	C5A-C6A-N6A	2.30	123.85	120.35
2	B	501	FAD	C5A-C6A-N6A	2.30	123.84	120.35
2	D	501	FAD	C5A-C6A-N6A	2.30	123.84	120.35
2	E	501	FAD	C5A-C6A-N6A	2.30	123.84	120.35
2	A	501	FAD	C5A-C6A-N6A	2.29	123.84	120.35
2	G	501	FAD	C5A-C6A-N6A	2.28	123.82	120.35
2	C	501	FAD	C5A-C6A-N6A	2.24	123.76	120.35

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3B-C4B-C5B-O5B
2	C	501	FAD	C5B-O5B-PA-O1A
2	C	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	C5B-O5B-PA-O3P
2	C	501	FAD	C5'-O5'-P-O2P
2	C	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	C5B-O5B-PA-O2A
2	D	501	FAD	O4B-C4B-C5B-O5B
2	E	501	FAD	C5B-O5B-PA-O1A
2	E	501	FAD	C5B-O5B-PA-O2A
2	G	501	FAD	C5B-O5B-PA-O1A
2	G	501	FAD	C5B-O5B-PA-O2A
2	G	501	FAD	C5'-O5'-P-O3P
2	H	501	FAD	C5B-O5B-PA-O1A
2	H	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	O4B-C4B-C5B-O5B
2	E	501	FAD	O4B-C4B-C5B-O5B
2	E	501	FAD	C3B-C4B-C5B-O5B
2	F	501	FAD	O4B-C4B-C5B-O5B
2	G	501	FAD	O4B-C4B-C5B-O5B
2	G	501	FAD	C3B-C4B-C5B-O5B
2	H	501	FAD	O4B-C4B-C5B-O5B
2	H	501	FAD	C3B-C4B-C5B-O5B
2	D	501	FAD	C3B-C4B-C5B-O5B
2	F	501	FAD	C3B-C4B-C5B-O5B
2	C	501	FAD	C2'-C3'-C4'-O4'
2	C	501	FAD	O3'-C3'-C4'-O4'
2	C	501	FAD	C2'-C3'-C4'-C5'
2	C	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	C2'-C3'-C4'-O4'
2	C	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	O3'-C3'-C4'-O4'
2	B	501	FAD	C2'-C3'-C4'-C5'
2	B	501	FAD	PA-O3P-P-O5'
2	G	501	FAD	P-O3P-PA-O5B
2	C	501	FAD	C5'-O5'-P-O3P
2	D	501	FAD	C5B-O5B-PA-O3P
2	E	501	FAD	C5B-O5B-PA-O3P
2	C	501	FAD	C5'-O5'-P-O1P

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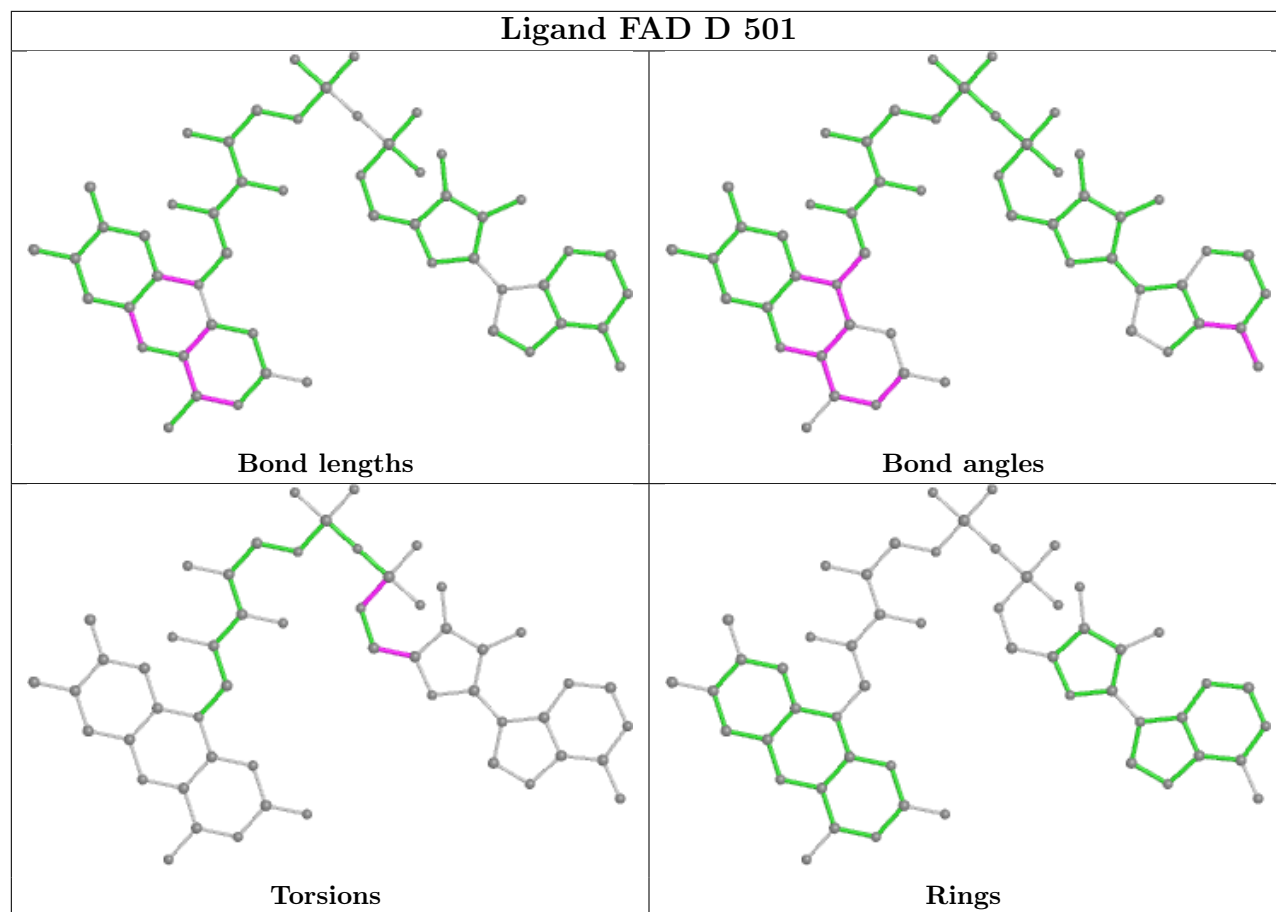
Mol	Chain	Res	Type	Atoms
2	D	501	FAD	C5B-O5B-PA-O1A
2	B	501	FAD	P-O3P-PA-O1A
2	F	501	FAD	C2'-C3'-C4'-O4'
2	A	501	FAD	C5B-O5B-PA-O3P
2	A	501	FAD	C5'-O5'-P-O3P
2	B	501	FAD	C5'-O5'-P-O3P
2	G	501	FAD	C5B-O5B-PA-O3P
2	H	501	FAD	C5B-O5B-PA-O3P
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	PA-O3P-P-O2P
2	C	501	FAD	PA-O3P-P-O2P
2	G	501	FAD	PA-O3P-P-O2P
2	B	501	FAD	C5'-O5'-P-O1P
2	G	501	FAD	C5'-O5'-P-O1P
2	G	501	FAD	C5'-O5'-P-O2P

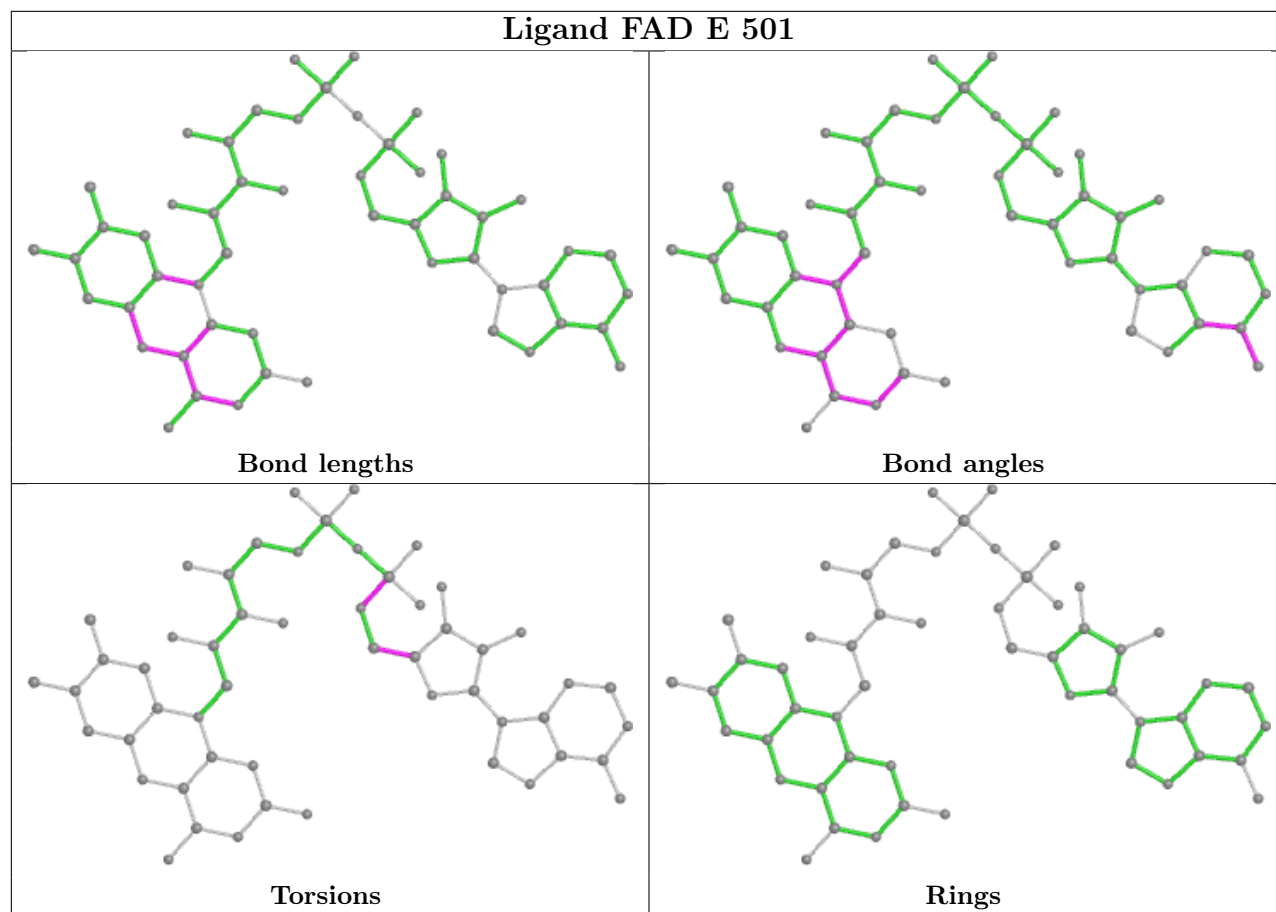
There are no ring outliers.

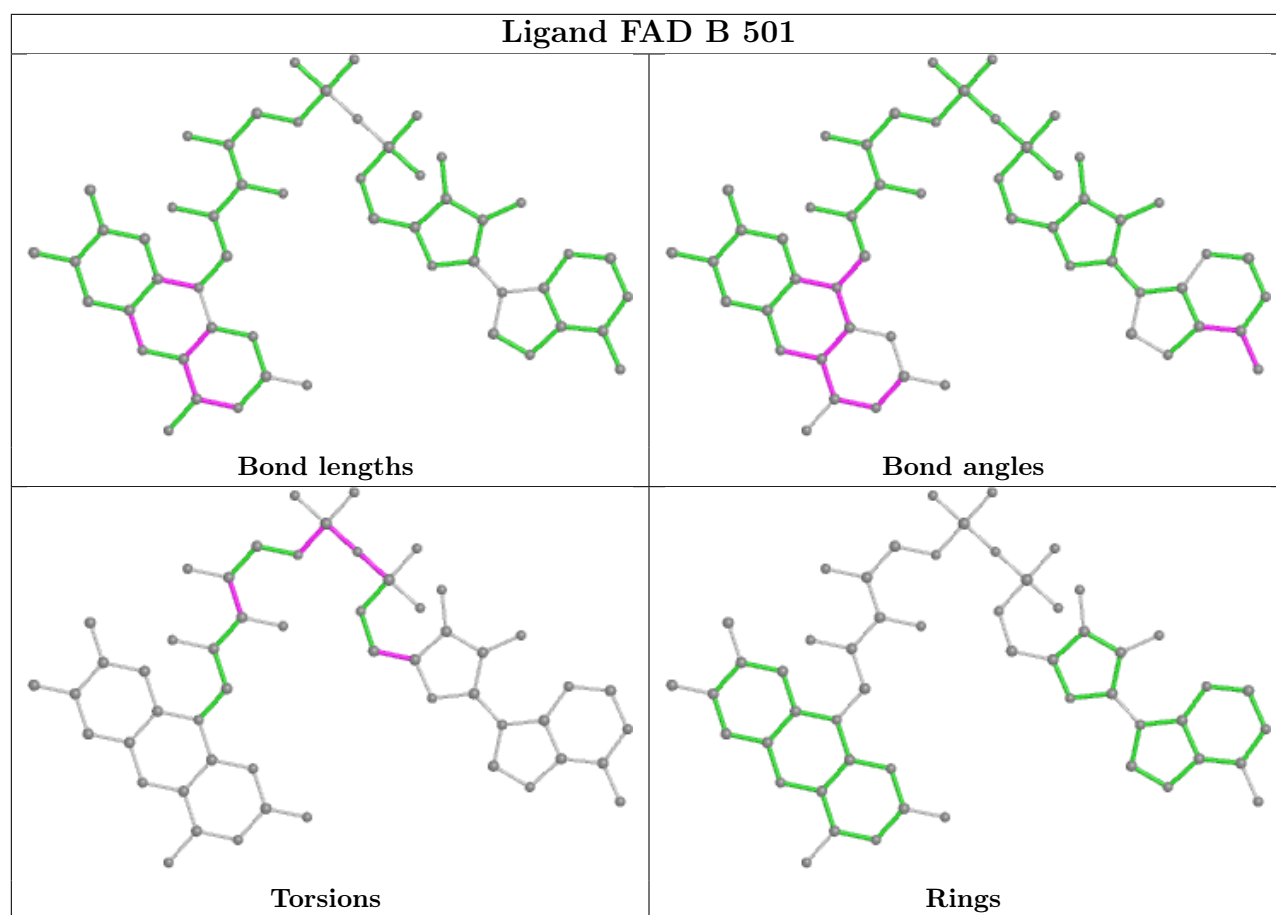
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FAD	3	0
2	E	501	FAD	2	0
2	B	501	FAD	1	0
2	H	501	FAD	2	0
2	G	501	FAD	2	0
2	A	501	FAD	1	0
2	C	501	FAD	2	0

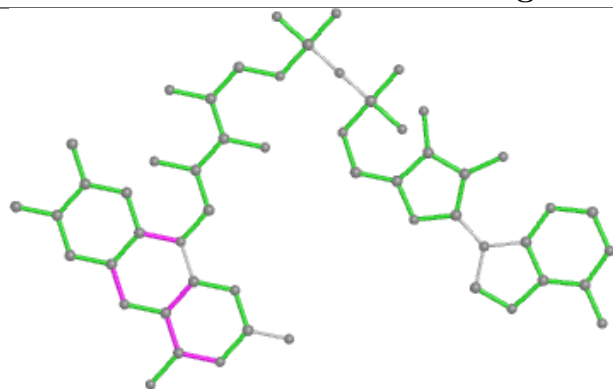
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



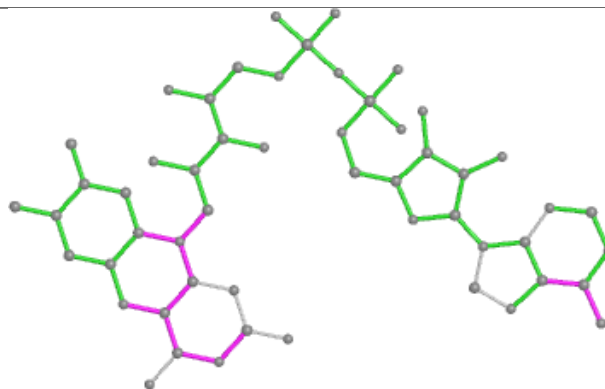




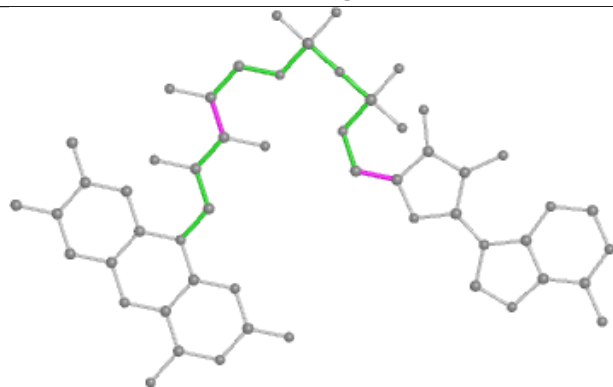
## Ligand FAD F 501



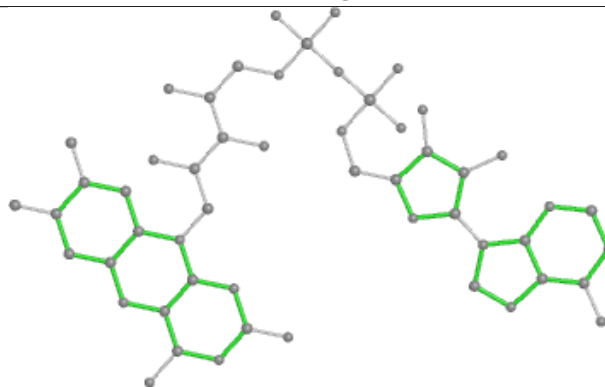
Bond lengths



Bond angles

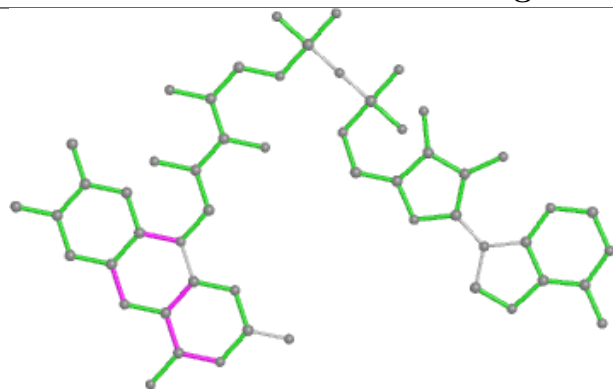


Torsions

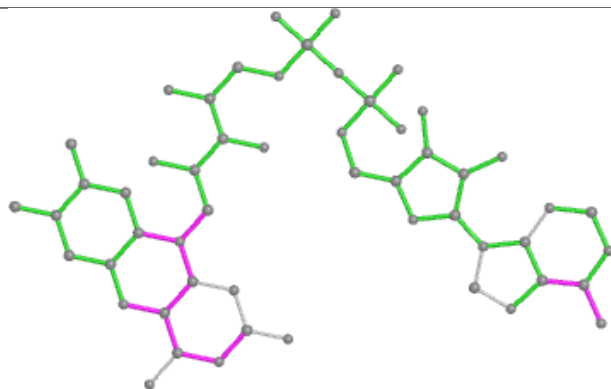


Rings

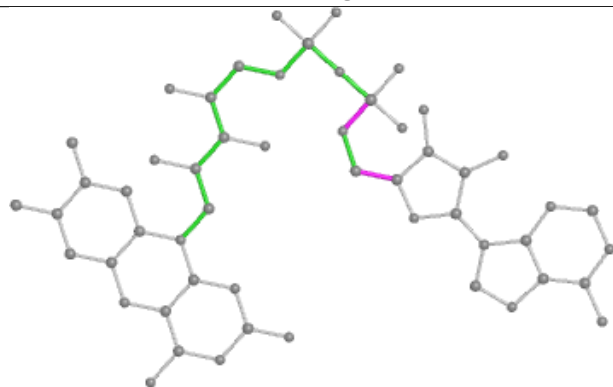
## Ligand FAD H 501



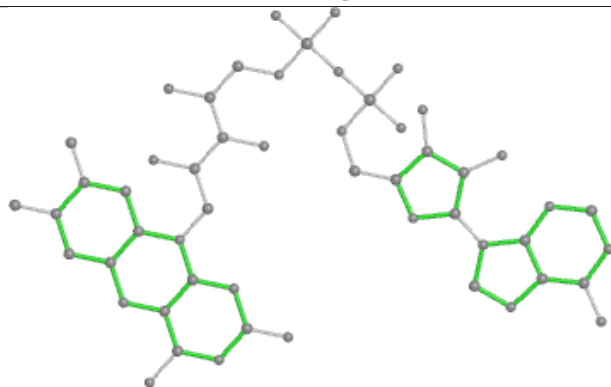
Bond lengths



Bond angles

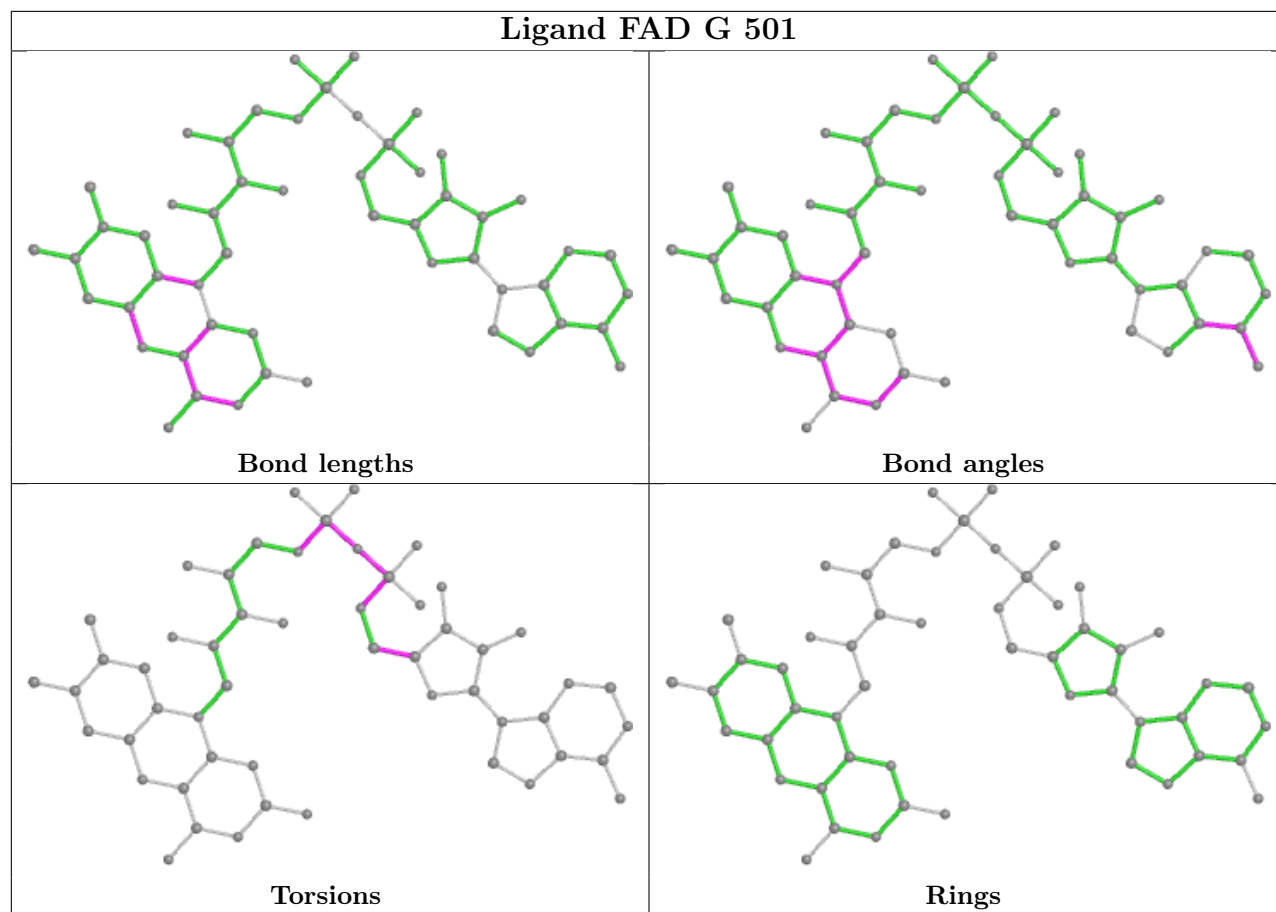


Torsions

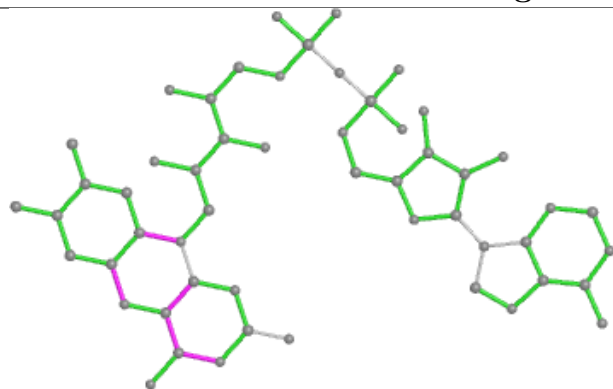


Rings

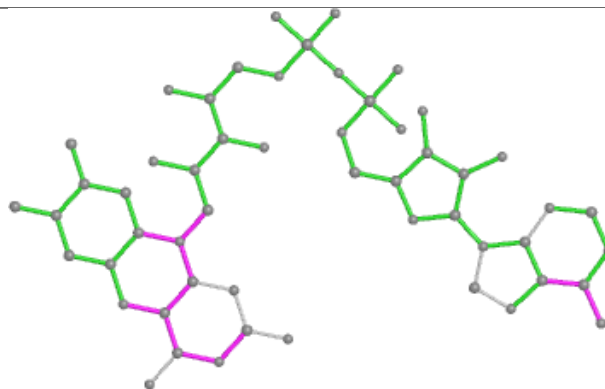




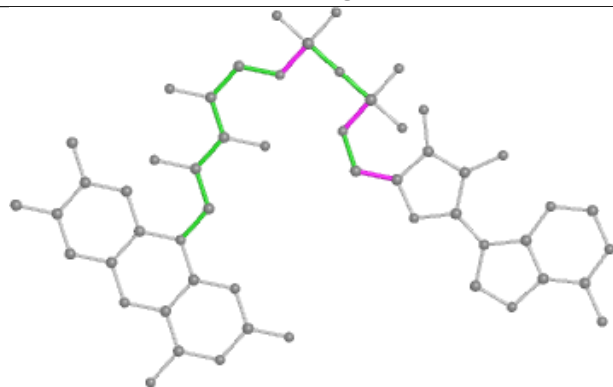
## Ligand FAD A 501



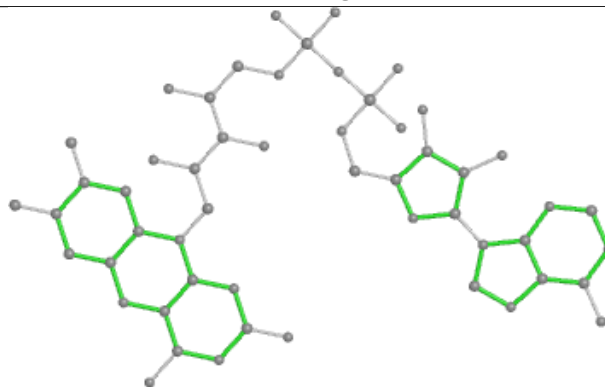
Bond lengths



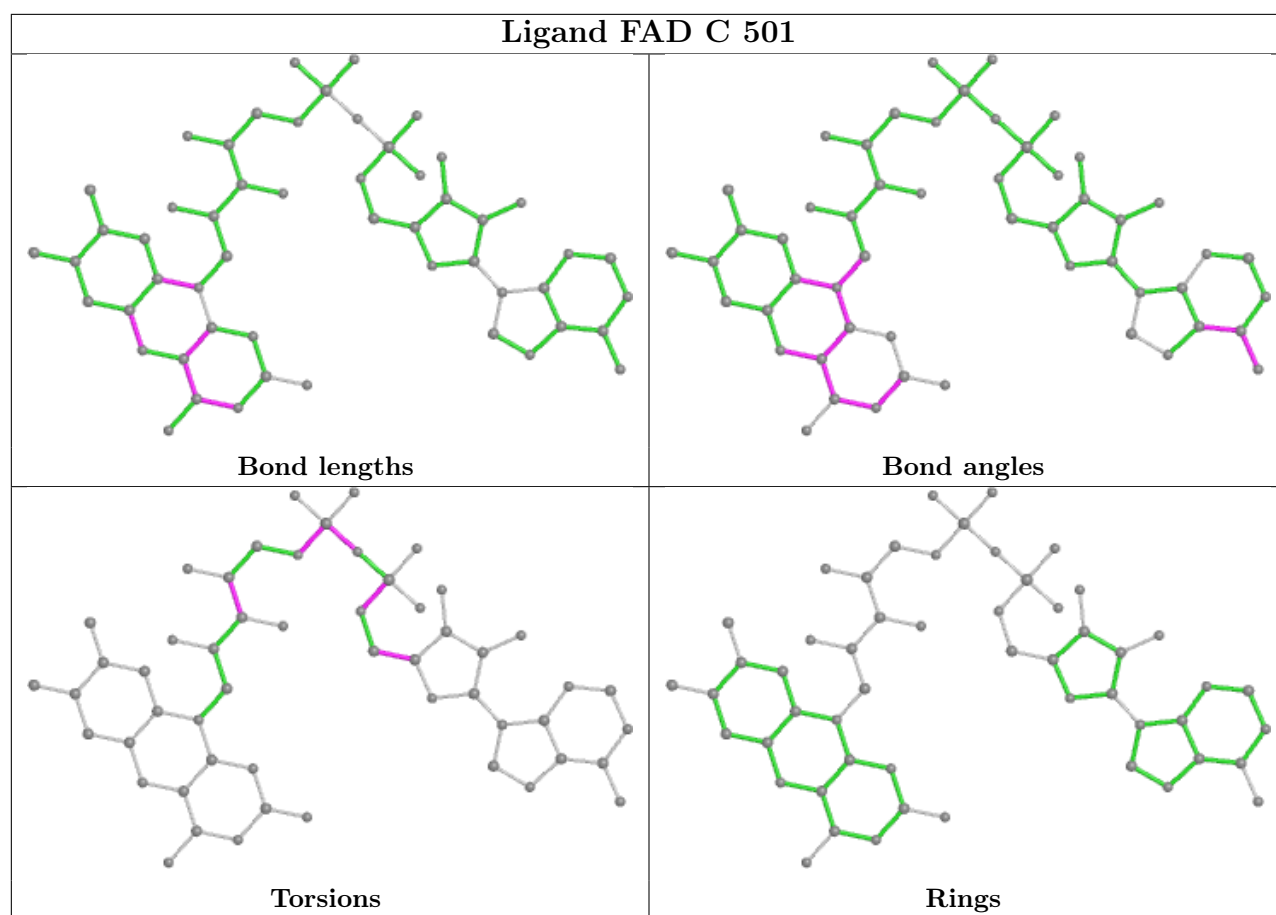
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	416/425 (97%)	-0.27	2 (0%) 91 90	19, 42, 71, 92	0
1	B	416/425 (97%)	-0.12	3 (0%) 87 87	23, 51, 75, 92	0
1	C	414/425 (97%)	-0.03	7 (1%) 70 68	28, 52, 76, 87	0
1	D	414/425 (97%)	0.04	7 (1%) 70 68	27, 55, 79, 96	0
1	E	416/425 (97%)	-0.27	4 (0%) 82 81	17, 39, 66, 83	0
1	F	415/425 (97%)	-0.04	9 (2%) 62 59	24, 48, 75, 95	0
1	G	418/425 (98%)	-0.12	6 (1%) 75 74	21, 46, 72, 84	0
1	H	416/425 (97%)	-0.20	3 (0%) 87 87	20, 41, 64, 85	0
All	All	3325/3400 (97%)	-0.13	41 (1%) 79 78	17, 47, 74, 96	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	425	VAL	6.6
1	F	340	ALA	3.5
1	D	126	VAL	3.5
1	F	313	LEU	3.3
1	F	134	ASP	3.3
1	F	360	PHE	3.3
1	E	127	THR	3.3
1	F	132	GLU	3.1
1	D	308	ASN	2.9
1	F	135	LEU	2.9
1	A	35	GLU	2.8
1	E	308	ASN	2.8
1	C	368	ILE	2.8
1	B	340	ALA	2.7
1	D	307	GLU	2.7
1	F	326	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	165	CYS	2.6
1	F	133	ASP	2.5
1	E	142	ALA	2.4
1	G	335	THR	2.4
1	C	185	LEU	2.4
1	D	142	ALA	2.4
1	H	142	ALA	2.3
1	D	138	VAL	2.3
1	C	267	PHE	2.3
1	B	141	SER	2.3
1	G	268	LYS	2.3
1	A	365	ALA	2.3
1	F	381	GLY	2.2
1	D	153	LEU	2.2
1	E	407	LEU	2.2
1	G	165	CYS	2.2
1	C	301	LEU	2.1
1	G	302	ASN	2.1
1	H	375	VAL	2.1
1	G	255	THR	2.1
1	C	425	VAL	2.1
1	C	12	HIS	2.1
1	D	125	THR	2.1
1	B	153	LEU	2.1
1	H	308	ASN	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 ⓘ

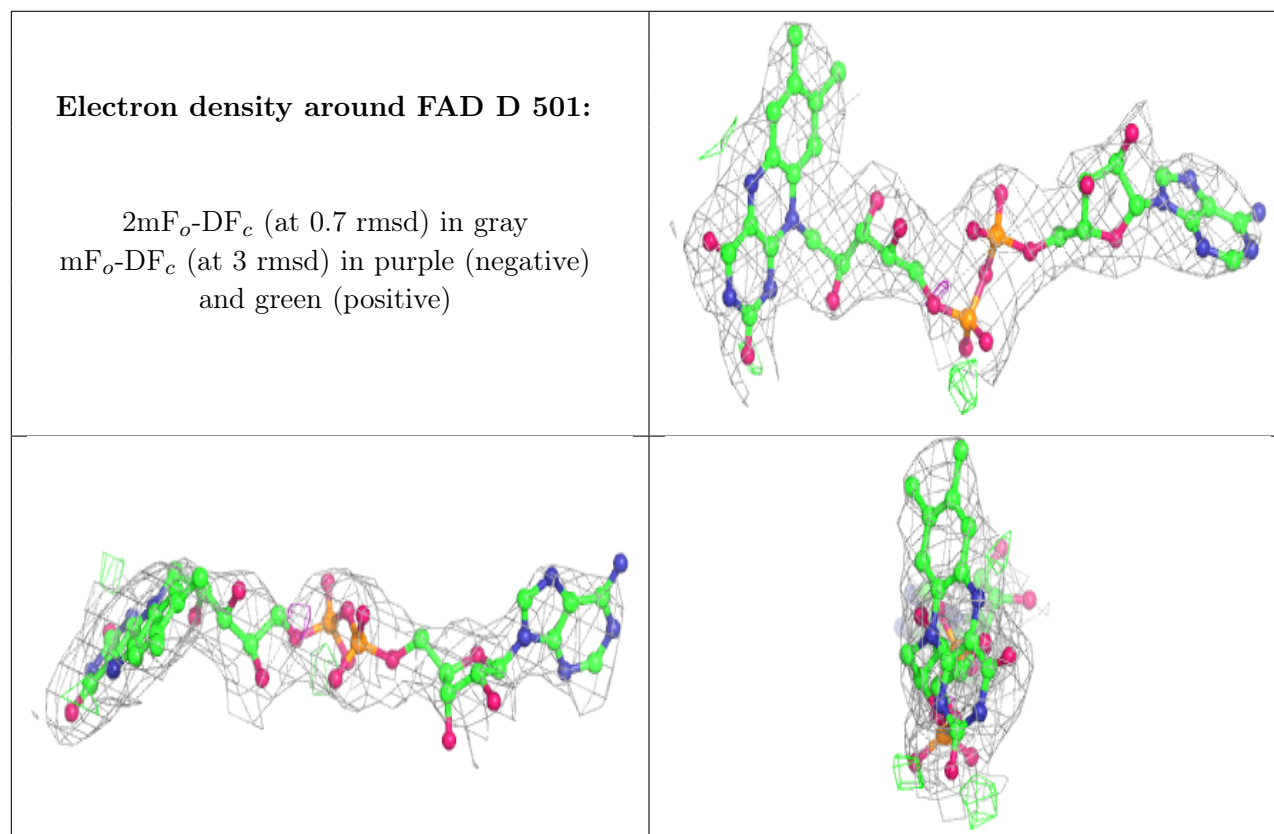
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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.

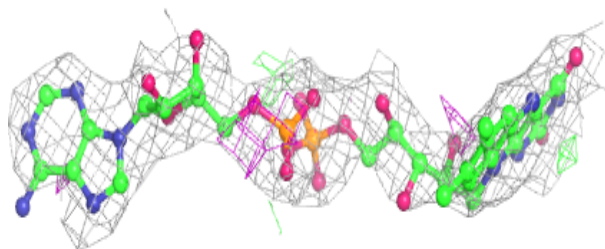
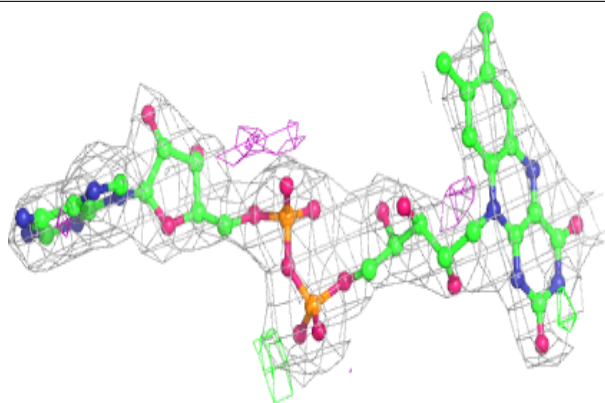
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	D	501	53/53	0.90	0.20	40,58,82,86	0
2	FAD	B	501	53/53	0.93	0.20	38,49,59,65	0
2	FAD	C	501	53/53	0.94	0.15	32,58,70,77	0
2	FAD	A	501	53/53	0.94	0.17	25,40,52,58	0
2	FAD	F	501	53/53	0.94	0.17	38,55,70,73	0
2	FAD	G	501	53/53	0.94	0.17	31,49,68,79	0
2	FAD	H	501	53/53	0.95	0.17	23,38,50,55	0
2	FAD	E	501	53/53	0.96	0.14	21,34,52,56	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.

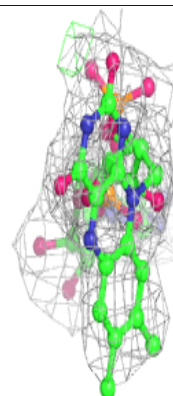
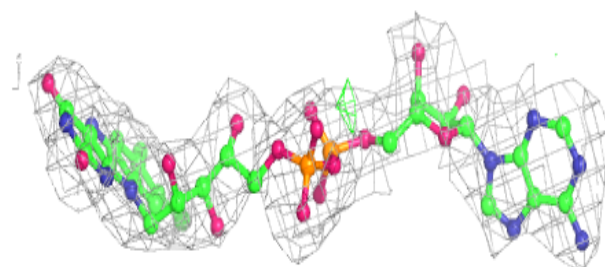
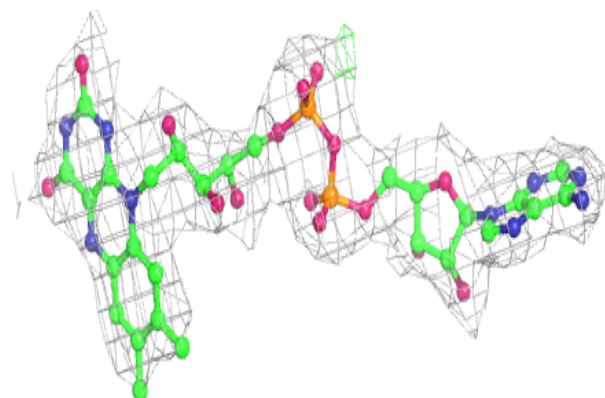


**Electron density around FAD B 501:**

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

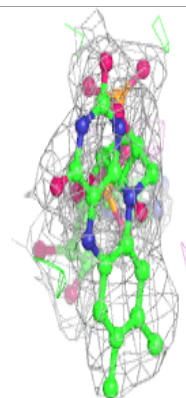
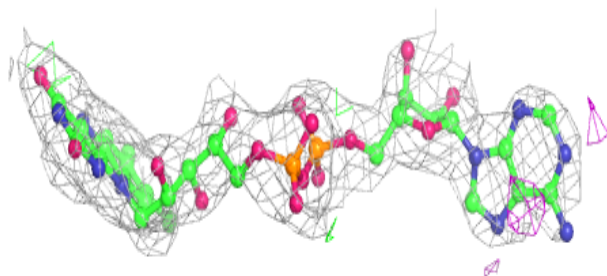
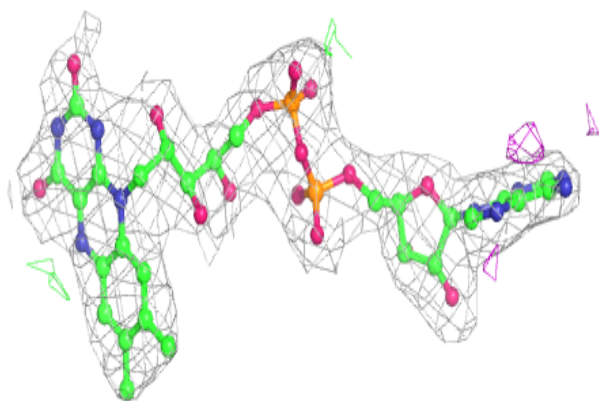
**Electron density around FAD C 501:**

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

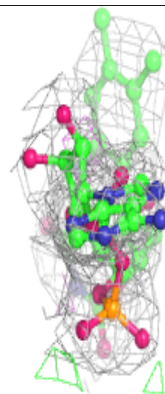
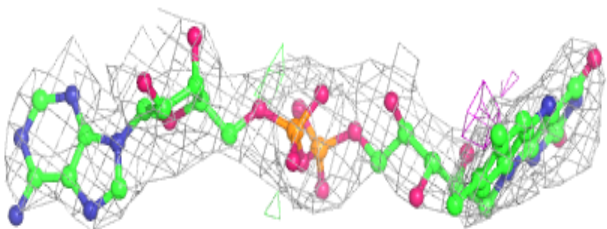
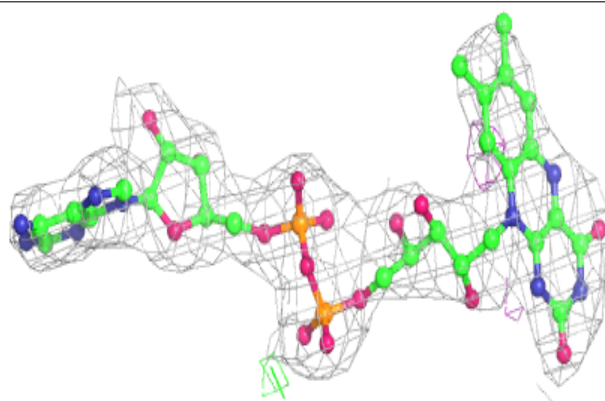


**Electron density around FAD A 501:**

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

**Electron density around FAD F 501:**

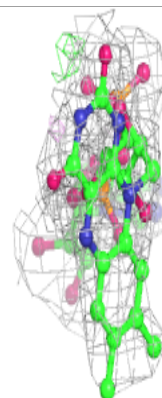
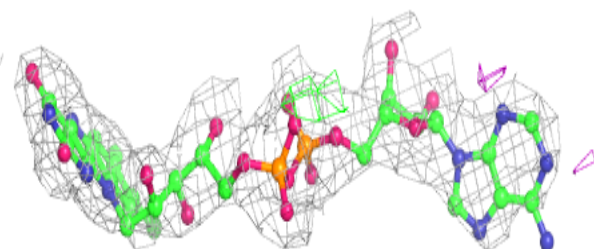
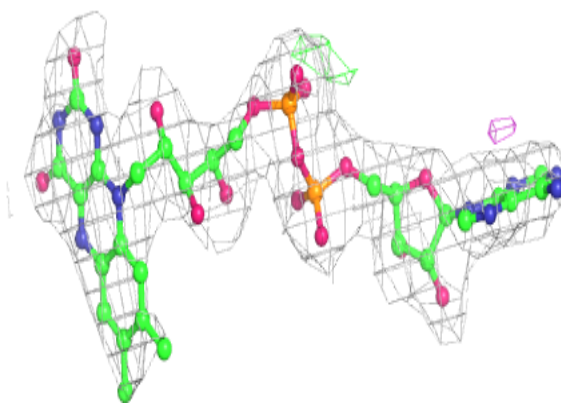
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



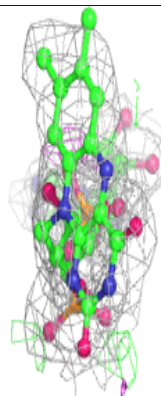
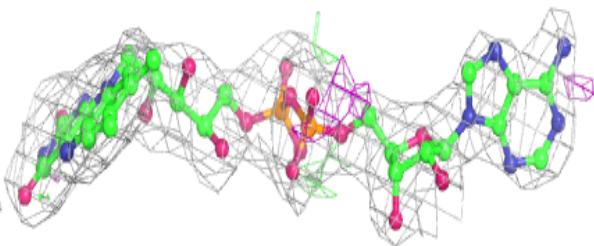
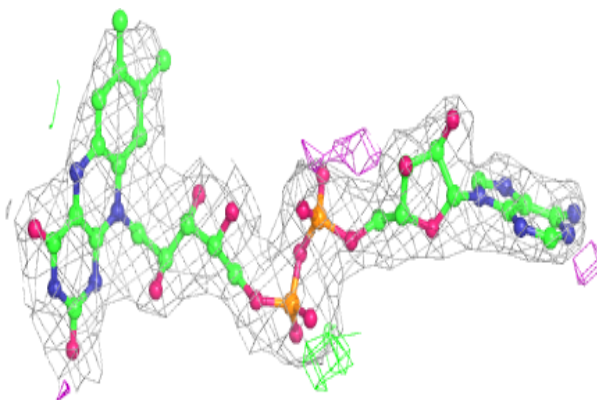


**Electron density around FAD G 501:**

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

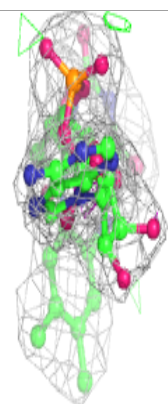
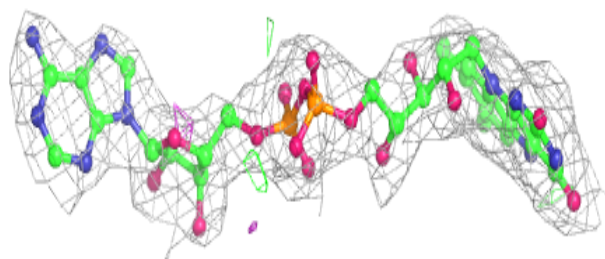
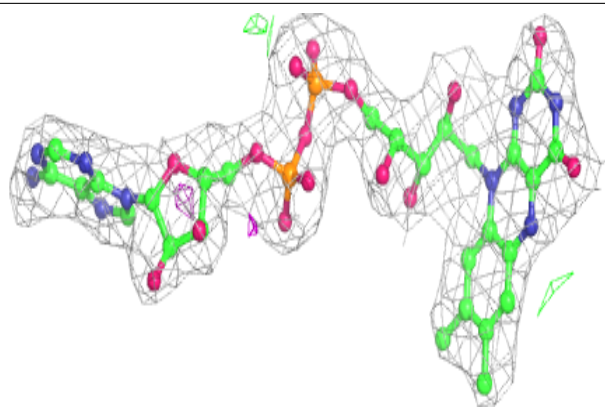
**Electron density around FAD H 501:**

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



**Electron density around FAD E 501:**

$2mF_o - DF_c$  (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.