



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 03:19 PM EDT

PDB ID : 2A1T  
Title : Structure of the human MCAD:ETF E165betaA complex  
Authors : Toogood, H.S.; Van Thiel, A.; Scrutton, N.S.; Leys, D.  
Deposited on : 2005-06-21  
Resolution : 2.80 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

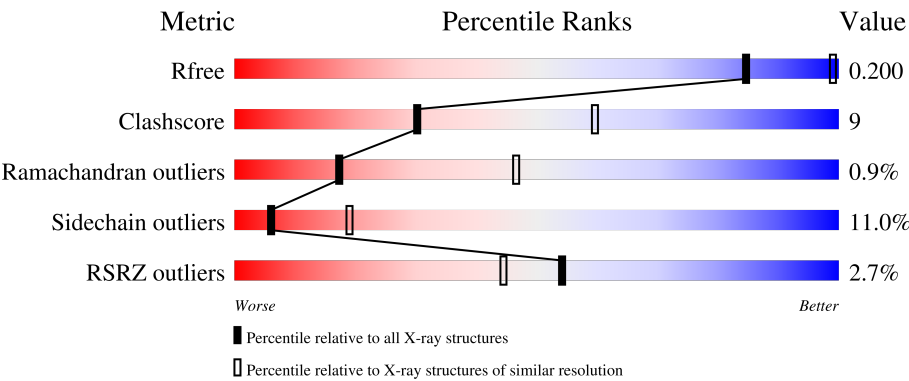
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	421	<div><div></div><div>68%21%• 8%</div></div>
1	B	421	<div><div></div><div>69%21%• 8%</div></div>
1	C	421	<div><div></div><div>72%18%• 8%</div></div>
1	D	421	<div><div>%</div><div>68%20%• 8%</div></div>
2	R	333	<div><div>12%</div><div>67%23%• 6%</div></div>

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Mol	Chain	Length	Quality of chain
3	S	255	<div><div></div><div>4%</div><div>68%</div><div>22%</div><div>6%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16189 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 Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2933	1862	496	557	18			
1	B	387	Total	C	N	O	S	0	0	0
			2949	1869	501	561	18			
1	C	388	Total	C	N	O	S	0	0	0
			2961	1875	508	560	18			
1	D	387	Total	C	N	O	S	0	0	0
			2972	1880	508	566	18			

- Molecule 2 is a protein called Electron transfer flavoprotein alpha-subunit, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	313	Total	C	N	O	S	0	0	0
			2264	1441	377	437	9			

- Molecule 3 is a protein called Electron transfer flavoprotein beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	239	Total	C	N	O	S	0	0	0
			1758	1119	294	337	8			

There is a discrepancy between the modelled and reference sequences:

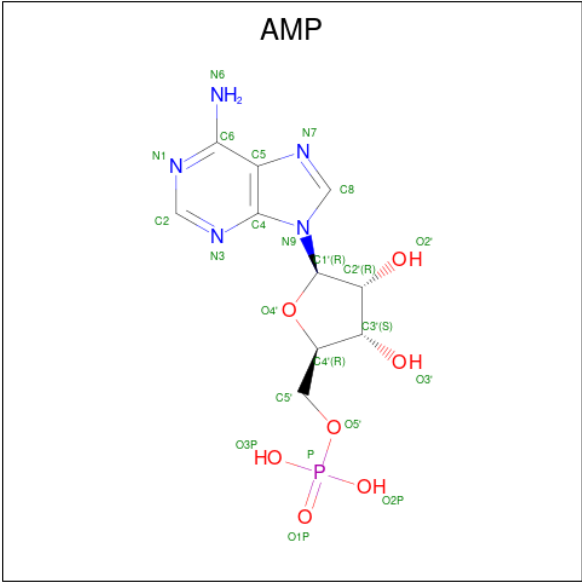
Chain	Residue	Modelled	Actual	Comment	Reference
S	165	ALA	GLU	engineered mutation	UNP P38117

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	R	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

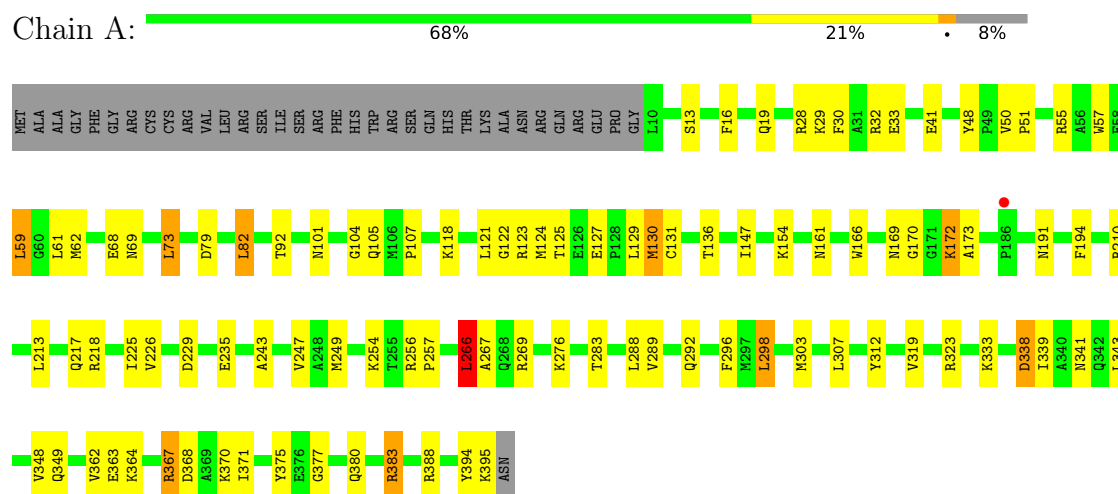
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	9	Total	O	0	0
			9	9		
6	C	17	Total	O	0	0
			17	17		
6	D	12	Total	O	0	0
			12	12		
6	R	3	Total	O	0	0
			3	3		
6	S	10	Total	O	0	0
			10	10		

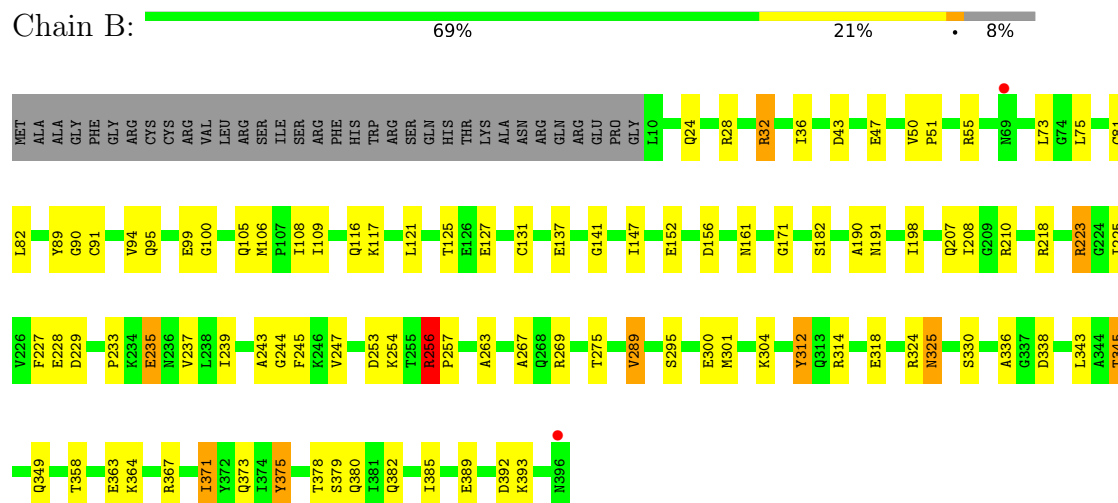
### 3 Residue-property plots

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: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

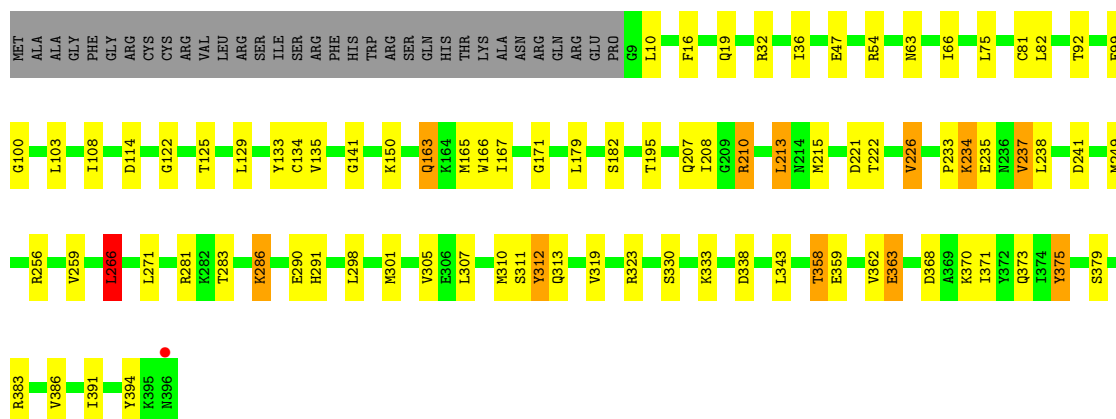


- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

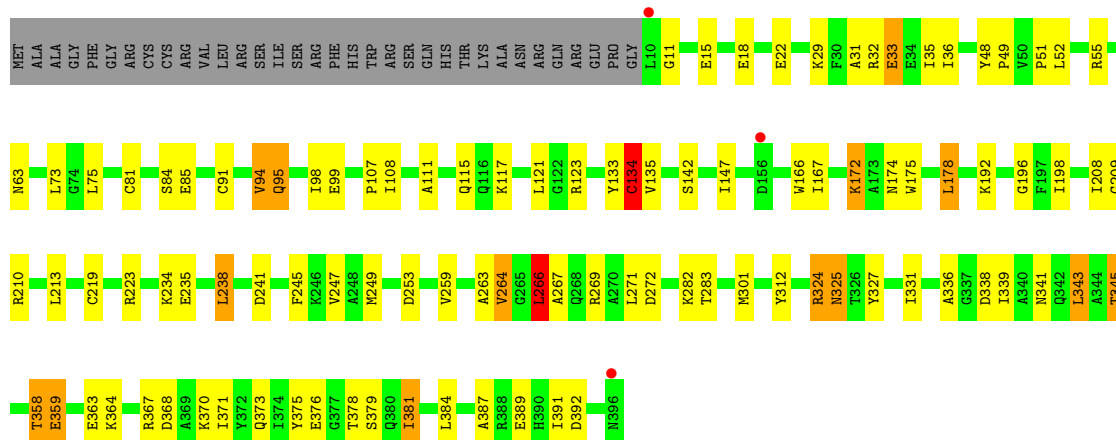


- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

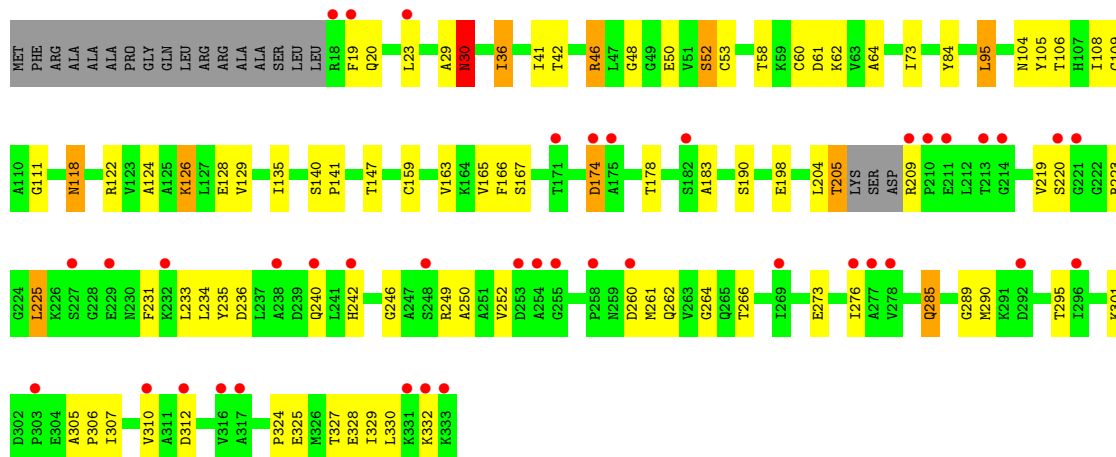




- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

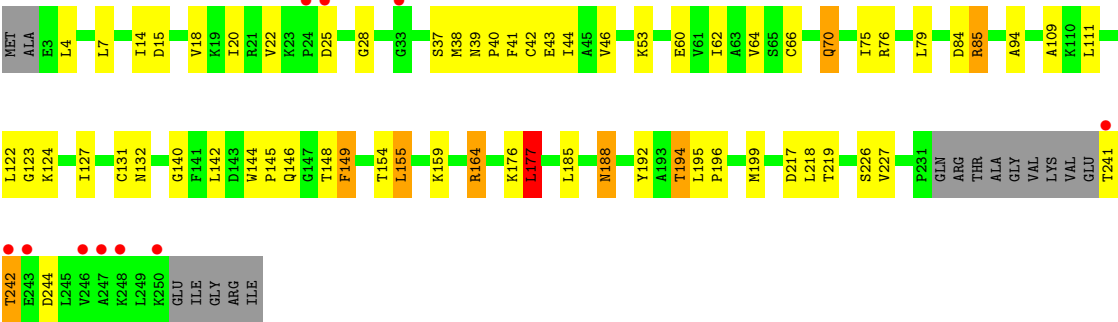


- Molecule 2: Electron transfer flavoprotein alpha-subunit, mitochondrial precursor



- Molecule 3: Electron transfer flavoprotein beta-subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.18Å 100.66Å 244.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.80) 93.0 (19.98-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0011	Depositor
R, $R_{free}$	0.199 , 0.269 0.205 , 0.200	Depositor DCC
$R_{free}$ test set	2734 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.74	1/2988 (0.0%)	0.83	6/4040 (0.1%)
1	B	0.76	0/3004	0.80	1/4062 (0.0%)
1	C	0.73	0/3016	0.83	3/4074 (0.1%)
1	D	0.72	1/3027 (0.0%)	0.81	1/4085 (0.0%)
2	R	0.63	0/2298	0.73	1/3129 (0.0%)
3	S	0.68	2/1778 (0.1%)	0.77	1/2417 (0.0%)
All	All	0.72	4/16111 (0.0%)	0.80	13/21807 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
3	S	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	66	CYS	CB-SG	-5.89	1.72	1.81
3	S	131	CYS	CB-SG	-5.59	1.72	1.81
1	D	134	CYS	CB-SG	-5.39	1.73	1.81
1	A	41	GLU	CG-CD	5.04	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH1	7.56	124.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	388	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	388	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	256	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	266	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	266	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	338	ASP	CB-CG-OD1	5.52	123.27	118.30
2	R	46	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	266	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	367	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	383	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	S	177	LEU	C-N-CD	5.17	139.25	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	325	ASN	Peptide
3	S	176	LYS	Peptide
3	S	177	LEU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2855	57	0
1	B	2949	0	2862	60	0
1	C	2961	0	2903	50	0
1	D	2972	0	2916	63	0
2	R	2264	0	2268	50	0
3	S	1758	0	1795	42	0
4	A	53	0	31	7	0
4	B	53	0	31	3	0
4	C	53	0	31	5	0
4	D	53	0	31	4	0
4	R	53	0	31	4	0
5	S	23	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	13	0	0	3	0
6	B	9	0	0	0	0
6	C	17	0	0	2	0
6	D	12	0	0	3	0
6	R	3	0	0	1	0
6	S	10	0	0	0	0
All	All	16189	0	15766	298	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 9.

All (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:THR:HG21	4:B:1399:FAD:O2B	1.51	1.07
2:R:84:TYR:OH	2:R:95:LEU:HD23	1.71	0.91
1:A:341:ASN:HD21	1:A:370:LYS:HA	1.40	0.85
1:B:116:GLN:NE2	1:B:237:VAL:O	2.09	0.84
6:D:3411:HOH:O	2:R:266:THR:HG21	1.78	0.84
3:S:39:ASN:ND2	3:S:127:ILE:HG12	1.92	0.84
1:C:213:LEU:O	1:D:358:THR:HB	1.79	0.82
3:S:39:ASN:HD22	3:S:127:ILE:HG12	1.43	0.81
6:A:411:HOH:O	1:B:345:THR:HG21	1.90	0.72
1:D:259:VAL:HG21	1:D:376:GLU:HG3	1.69	0.71
3:S:28:GLY:HA2	3:S:227:VAL:HG21	1.70	0.71
1:D:325:ASN:HD22	1:D:325:ASN:H	1.36	0.71
2:R:61:ASP:HA	2:R:64:ALA:HB3	1.73	0.70
1:A:380:GLN:NE2	4:A:399:FAD:O2B	2.25	0.70
1:C:234:LYS:O	1:C:237:VAL:HG12	1.94	0.68
1:B:253:ASP:O	1:B:325:ASN:ND2	2.27	0.67
3:S:177:LEU:HD23	3:S:177:LEU:O	1.94	0.67
3:S:124:LYS:O	3:S:132:ASN:ND2	2.27	0.67
2:R:122:ARG:HH11	3:S:146:GLN:HE21	1.42	0.67
1:D:387:ALA:O	1:D:391:ILE:HG12	1.95	0.66
1:D:108:ILE:HD12	1:D:175:TRP:CH2	2.32	0.65
1:C:171:GLY:HA2	1:C:208:ILE:HD13	1.77	0.64
1:A:364:LYS:HA	1:A:367:ARG:NH1	2.13	0.64
1:C:358:THR:HB	1:D:213:LEU:O	1.96	0.64
1:D:208:ILE:CG2	1:D:223:ARG:HD2	2.29	0.62
2:R:23:LEU:HA	2:R:52:SER:O	1.99	0.61
1:B:256:ARG:CG	1:B:256:ARG:HH11	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLU:OE2	1:B:147:ILE:HB	2.01	0.60
1:C:108:ILE:N	1:C:108:ILE:HD12	2.16	0.60
2:R:46:ARG:HG2	2:R:46:ARG:HH11	1.67	0.59
1:C:207:GLN:HB2	1:C:226:VAL:HG13	1.84	0.59
1:A:333:LYS:NZ	1:A:377:GLY:O	2.36	0.59
1:C:338:ASP:HA	1:C:373:GLN:HE21	1.68	0.59
1:A:123:ARG:HG3	1:A:124:MET:HE2	1.84	0.59
1:C:333:LYS:NZ	1:C:375:TYR:O	2.28	0.59
1:A:131:CYS:HA	1:A:173:ALA:HB1	1.85	0.58
1:B:314:ARG:NH1	1:B:318:GLU:OE2	2.36	0.58
2:R:122:ARG:HH11	3:S:146:GLN:NE2	2.01	0.58
1:A:371:ILE:CD1	4:A:399:FAD:HM83	2.34	0.58
1:B:28:ARG:O	1:B:32:ARG:HG2	2.04	0.58
1:D:18:GLU:O	1:D:22:GLU:HG3	2.03	0.58
1:B:363:GLU:OE2	1:B:367:ARG:NE	2.36	0.57
2:R:329:ILE:HD12	3:S:242:THR:HG23	1.87	0.57
2:R:220:SER:HA	2:R:246:GLY:O	2.05	0.57
1:D:378:THR:HG23	6:D:3402:HOH:O	2.04	0.57
1:D:271:LEU:HD13	1:D:301:MET:HB3	1.86	0.56
2:R:36:ILE:HG12	2:R:111:GLY:HA3	1.87	0.56
3:S:159:LYS:C	3:S:177:LEU:HD12	2.25	0.56
1:A:394:TYR:OH	1:D:272:ASP:OD1	2.18	0.56
1:C:133:TYR:CE2	1:C:135:VAL:HG21	2.40	0.56
1:A:371:ILE:HD11	4:A:399:FAD:HM83	1.88	0.56
1:A:101:ASN:HD21	1:A:130:MET:HA	1.71	0.56
2:R:124:ALA:O	2:R:128:GLU:N	2.39	0.56
1:C:310:MET:HA	1:C:313:GLN:HE21	1.71	0.55
1:D:81:CYS:HB3	1:D:312:TYR:CE1	2.42	0.55
1:B:233:PRO:CB	1:B:235:GLU:HG2	2.36	0.55
3:S:60:GLU:OE2	3:S:85:ARG:HD3	2.06	0.55
3:S:177:LEU:O	3:S:177:LEU:CD2	2.55	0.55
1:A:16:PHE:CE2	1:A:82:LEU:HD21	2.41	0.55
1:C:166:TRP:O	4:C:2399:FAD:C4X	2.54	0.55
1:D:266:LEU:C	1:D:266:LEU:HD12	2.27	0.55
1:B:267:ALA:HB1	1:B:343:LEU:HD22	1.89	0.55
2:R:126:LYS:NZ	3:S:140:GLY:O	2.35	0.55
2:R:262:GLN:NE2	2:R:266:THR:OG1	2.39	0.55
1:B:89:TYR:CE2	1:B:269:ARG:HA	2.42	0.55
1:D:29:LYS:O	1:D:33:GLU:HB2	2.07	0.55
1:D:133:TYR:CZ	1:D:135:VAL:HG21	2.42	0.55
2:R:73:ILE:O	2:R:183:ALA:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASP:HA	1:B:373:GLN:HE21	1.71	0.54
1:A:79:ASP:HA	1:A:82:LEU:HD12	1.88	0.54
1:B:190:ALA:HB1	1:B:245:PHE:CD1	2.42	0.54
1:D:135:VAL:HG13	1:D:147:ILE:HD11	1.88	0.54
1:C:32:ARG:HA	1:C:36:ILE:HD12	1.90	0.54
3:S:53:LYS:NZ	3:S:84:ASP:OD2	2.32	0.54
3:S:195:LEU:O	3:S:199:MET:HE3	2.06	0.54
1:A:73:LEU:HD12	1:A:73:LEU:H	1.71	0.54
1:B:161:ASN:ND2	1:B:229:ASP:H	2.05	0.54
1:B:32:ARG:NH1	1:B:89:TYR:CE1	2.76	0.53
1:A:341:ASN:HB3	6:A:411:HOH:O	2.06	0.53
1:B:378:THR:CG2	1:B:380:GLN:HE21	2.21	0.53
1:B:233:PRO:HB3	1:B:235:GLU:HG2	1.89	0.53
1:C:283:THR:HG22	6:C:2415:HOH:O	2.09	0.53
1:C:371:ILE:CD1	4:C:2399:FAD:HM83	2.38	0.53
1:D:209:GLY:O	1:D:223:ARG:HD3	2.08	0.53
1:A:123:ARG:HG3	1:A:124:MET:CE	2.38	0.53
1:B:208:ILE:HG12	1:B:225:ILE:HD12	1.91	0.53
1:D:371:ILE:CD1	4:D:3399:FAD:HM83	2.39	0.53
1:D:49:PRO:HB2	1:D:52:LEU:HD12	1.90	0.53
1:D:245:PHE:O	1:D:249:MET:HG2	2.09	0.53
1:A:213:LEU:O	1:B:358:THR:HB	2.09	0.53
2:R:305:ALA:O	2:R:307:ILE:N	2.42	0.52
3:S:194:THR:HG23	3:S:196:PRO:HD2	1.91	0.52
1:D:117:LYS:O	1:D:121:LEU:HB2	2.09	0.52
3:S:44:ILE:HG23	3:S:188:ASN:ND2	2.24	0.52
1:A:28:ARG:O	1:A:32:ARG:HG3	2.09	0.52
1:B:73:LEU:HB3	1:B:75:LEU:HD13	1.91	0.52
1:A:267:ALA:HB1	1:A:343:LEU:HD22	1.92	0.51
1:C:266:LEU:HD12	1:C:266:LEU:C	2.30	0.51
1:D:253:ASP:HA	1:D:325:ASN:HD21	1.76	0.51
1:A:370:LYS:NZ	1:B:349:GLN:HE21	2.06	0.51
1:B:300:GLU:O	1:B:304:LYS:HG3	2.09	0.51
1:C:368:ASP:O	1:C:371:ILE:HG22	2.10	0.51
1:D:32:ARG:HA	1:D:36:ILE:HD12	1.92	0.51
1:A:29:LYS:O	1:A:33:GLU:HB2	2.10	0.51
2:R:325:GLU:O	2:R:329:ILE:HG13	2.10	0.51
3:S:7:LEU:HD12	3:S:62:ILE:HB	1.93	0.51
2:R:231:PHE:CD2	2:R:234:LEU:HD12	2.45	0.51
1:C:371:ILE:HD13	4:C:2399:FAD:HM83	1.92	0.50
1:A:13:SER:HB3	1:D:11:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:HH11	1:B:256:ARG:HG3	1.76	0.50
2:R:41:ILE:HG21	2:R:73:ILE:HD11	1.93	0.50
2:R:260:ASP:OD1	2:R:260:ASP:N	2.44	0.50
1:A:349:GLN:HE22	1:B:373:GLN:HB3	1.76	0.50
1:C:210:ARG:NE	2:R:249:ARG:HH21	2.09	0.50
1:C:234:LYS:O	1:C:237:VAL:CG1	2.58	0.50
1:B:378:THR:HG21	1:B:380:GLN:HE21	1.77	0.50
2:R:124:ALA:HB1	2:R:129:VAL:O	2.11	0.50
3:S:14:ILE:N	3:S:14:ILE:HD12	2.27	0.50
1:B:301:MET:HG2	1:B:343:LEU:HG	1.94	0.50
2:R:285:GLN:NE2	4:R:599:FAD:O2'	2.45	0.50
3:S:40:PRO:HA	3:S:43:GLU:HG3	1.93	0.50
1:A:256:ARG:N	1:A:257:PRO:CD	2.75	0.50
1:A:338:ASP:OD2	1:A:383:ARG:NH2	2.42	0.49
1:B:81:CYS:HB3	1:B:312:TYR:CE1	2.48	0.49
2:R:73:ILE:O	2:R:183:ALA:CB	2.60	0.49
1:A:296:PHE:HE1	1:D:384:LEU:HD21	1.77	0.49
2:R:41:ILE:CG2	2:R:73:ILE:HD11	2.41	0.49
2:R:140:SER:HB2	2:R:141:PRO:CD	2.42	0.49
3:S:44:ILE:HA	3:S:188:ASN:HD21	1.76	0.49
2:R:109:CYS:HB2	2:R:166:PHE:O	2.11	0.49
1:B:378:THR:HG21	4:B:1399:FAD:HO2A	1.70	0.49
1:C:233:PRO:O	1:C:235:GLU:N	2.46	0.49
1:D:31:ALA:HA	1:D:35:ILE:HD12	1.94	0.49
1:B:289:VAL:HG22	1:C:391:ILE:CD1	2.43	0.48
1:A:368:ASP:O	1:A:371:ILE:HG22	2.13	0.48
1:A:105:GLN:HG2	1:A:121:LEU:HD22	1.95	0.48
1:B:371:ILE:CG2	4:B:1399:FAD:HM83	2.43	0.48
1:A:348:VAL:HG22	1:A:362:VAL:HG23	1.95	0.48
3:S:7:LEU:HD11	3:S:64:VAL:HG11	1.95	0.48
1:C:81:CYS:HB3	1:C:312:TYR:CE1	2.49	0.48
1:C:108:ILE:N	1:C:108:ILE:CD1	2.77	0.48
3:S:188:ASN:C	3:S:188:ASN:HD22	2.17	0.48
2:R:204:LEU:C	2:R:205:THR:HG23	2.34	0.48
2:R:301:LYS:HG2	4:R:599:FAD:C4A	2.44	0.47
1:A:92:THR:HB	1:A:217:GLN:OE1	2.14	0.47
1:B:24:GLN:HB2	1:B:82:LEU:HD13	1.96	0.47
1:D:107:PRO:O	1:D:111:ALA:N	2.47	0.47
1:A:30:PHE:HE1	1:A:55:ARG:HG2	1.79	0.47
1:C:16:PHE:CZ	1:C:82:LEU:HD21	2.50	0.47
1:C:63:ASN:HB3	1:C:66:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:CE2	1:A:172:LYS:HG2	2.50	0.47
4:A:399:FAD:H2'	4:A:399:FAD:H9	1.97	0.47
1:B:161:ASN:HD21	1:B:229:ASP:H	1.61	0.47
1:B:378:THR:O	1:B:382:GLN:HG2	2.14	0.47
1:D:91:CYS:HB3	1:D:94:VAL:HG13	1.97	0.47
2:R:61:ASP:OD1	2:R:62:LYS:N	2.48	0.47
1:C:134:CYS:HA	1:C:167:ILE:HD12	1.95	0.47
3:S:39:ASN:ND2	3:S:127:ILE:H	2.13	0.47
1:C:281:ARG:NH1	4:D:3399:FAD:O2A	2.47	0.47
1:C:163:GLN:HG2	6:R:602:HOH:O	2.15	0.46
1:C:312:TYR:CD1	1:C:312:TYR:C	2.88	0.46
2:R:42:THR:OG1	2:R:174:ASP:O	2.27	0.46
1:A:50:VAL:N	1:A:51:PRO:CD	2.79	0.46
3:S:4:LEU:HD11	3:S:155:LEU:HD21	1.96	0.46
3:S:4:LEU:N	3:S:4:LEU:HD23	2.30	0.46
1:D:51:PRO:O	1:D:55:ARG:HG2	2.15	0.46
1:C:215:MET:HB2	1:D:363:GLU:HG3	1.97	0.46
1:D:359:GLU:OE1	6:D:3411:HOH:O	2.20	0.46
3:S:70:GLN:NE2	3:S:70:GLN:N	2.63	0.46
1:A:370:LYS:HZ1	1:B:349:GLN:NE2	2.13	0.46
1:B:106:MET:HE3	1:B:109:ILE:HB	1.96	0.46
1:D:108:ILE:HD11	1:D:198:ILE:HG12	1.97	0.46
1:D:327:TYR:O	1:D:331:ILE:HG13	2.15	0.46
1:A:57:TRP:CZ2	1:A:127:GLU:HA	2.51	0.46
1:D:84:SER:HB2	1:D:95:GLN:OE1	2.16	0.46
1:A:292:GLN:NE2	4:D:3399:FAD:N1A	2.63	0.46
1:B:378:THR:CG2	1:B:380:GLN:NE2	2.78	0.46
1:B:43:ASP:HB2	1:B:364:LYS:HE2	1.99	0.45
1:B:378:THR:HG22	1:B:380:GLN:N	2.31	0.45
1:D:263:ALA:HB3	1:D:336:ALA:HB1	1.98	0.45
1:A:161:ASN:HD21	1:A:229:ASP:H	1.64	0.45
2:R:233:LEU:HD22	2:R:324:PRO:HG3	1.99	0.45
2:R:252:VAL:HG21	2:R:262:GLN:HB2	1.99	0.45
3:S:75:ILE:O	3:S:79:LEU:HG	2.15	0.45
1:A:50:VAL:N	1:A:51:PRO:HD2	2.31	0.45
1:D:338:ASP:HA	1:D:373:GLN:HE21	1.82	0.45
2:R:135:ILE:HG12	2:R:167:SER:O	2.17	0.45
2:R:29:ALA:O	2:R:30:ASN:C	2.56	0.45
2:R:108:ILE:O	2:R:165:VAL:HA	2.17	0.45
1:D:238:LEU:HD12	1:D:238:LEU:HA	1.82	0.44
1:D:238:LEU:HD23	1:D:247:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:399:FAD:H2'	4:A:399:FAD:C9	2.48	0.44
1:D:48:TYR:CE2	1:D:172:LYS:HG2	2.52	0.44
1:D:301:MET:HG2	1:D:343:LEU:HG	1.99	0.44
1:C:312:TYR:CD1	1:C:313:GLN:N	2.86	0.44
2:R:266:THR:HG23	4:R:599:FAD:N5	2.32	0.44
1:A:303:MET:HG2	1:D:331:ILE:HG23	1.99	0.44
1:B:243:ALA:O	1:B:247:VAL:HG13	2.18	0.44
1:C:286:LYS:HB3	1:C:290:GLU:OE1	2.18	0.44
1:B:161:ASN:HA	1:B:227:PHE:O	2.18	0.44
1:B:375:TYR:CD1	1:B:375:TYR:C	2.92	0.44
1:C:271:LEU:HD13	1:C:301:MET:HB3	2.00	0.44
3:S:28:GLY:HA2	3:S:227:VAL:CG2	2.45	0.44
1:C:210:ARG:HE	2:R:249:ARG:HH21	1.64	0.43
1:A:57:TRP:HB2	1:A:62:MET:HE3	2.00	0.43
2:R:324:PRO:O	2:R:328:GLU:HG2	2.18	0.43
1:A:123:ARG:HG3	1:A:129:LEU:HD12	1.99	0.43
1:C:16:PHE:CZ	1:C:82:LEU:CD2	3.01	0.43
1:A:136:THR:OG1	4:A:399:FAD:H1'1	2.18	0.43
1:A:266:LEU:C	1:A:266:LEU:HD12	2.37	0.43
1:C:122:GLY:O	1:C:125:THR:HB	2.19	0.43
1:D:253:ASP:CB	1:D:325:ASN:HD21	2.31	0.43
1:D:135:VAL:CG1	1:D:147:ILE:HD11	2.49	0.43
1:A:283:THR:HG23	1:A:288:LEU:HD21	2.00	0.43
1:B:235:GLU:CD	1:B:235:GLU:H	2.22	0.43
2:R:118:ASN:ND2	3:S:146:GLN:OE1	2.51	0.43
3:S:42:CYS:O	3:S:46:VAL:HG23	2.18	0.43
1:D:99:GLU:OE1	1:D:99:GLU:HA	2.19	0.43
3:S:149:PHE:CD1	3:S:149:PHE:N	2.86	0.43
1:A:147:ILE:HD11	1:A:194:PHE:CD1	2.54	0.43
1:A:166:TRP:O	4:A:399:FAD:C4X	2.66	0.43
1:D:301:MET:HA	1:D:343:LEU:HD11	2.01	0.43
1:B:233:PRO:HB2	1:B:235:GLU:HG2	2.01	0.43
1:C:362:VAL:O	1:C:363:GLU:C	2.56	0.43
2:R:23:LEU:HD22	2:R:105:TYR:CE2	2.54	0.43
3:S:41:PHE:HB3	3:S:123:GLY:HA3	2.01	0.43
1:D:73:LEU:HG	3:S:199:MET:HE1	2.01	0.42
1:B:50:VAL:N	1:B:51:PRO:CD	2.81	0.42
1:D:324:ARG:NH2	1:D:389:GLU:OE1	2.52	0.42
1:D:142:SER:HB3	1:D:381:ILE:HG21	2.01	0.42
1:D:364:LYS:HA	1:D:367:ARG:NH2	2.34	0.42
1:D:368:ASP:O	1:D:371:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:109:ALA:HA	3:S:142:LEU:HD21	2.01	0.42
1:A:254:LYS:HG2	1:A:319:VAL:HG21	2.01	0.42
1:B:105:GLN:HG3	1:B:131:CYS:SG	2.59	0.42
2:R:19:PHE:CG	2:R:19:PHE:O	2.72	0.42
1:A:104:GLY:O	1:A:107:PRO:HD2	2.20	0.42
1:A:55:ARG:O	1:A:59:LEU:HD22	2.20	0.42
1:C:319:VAL:HA	1:C:323:ARG:O	2.20	0.42
1:A:123:ARG:CG	1:A:124:MET:CE	2.98	0.42
1:A:169:ASN:O	1:A:170:GLY:C	2.58	0.42
2:R:30:ASN:HD22	2:R:30:ASN:HA	1.70	0.42
2:R:235:TYR:O	2:R:236:ASP:C	2.58	0.42
3:S:14:ILE:HD12	3:S:14:ILE:H	1.83	0.42
1:B:256:ARG:N	1:B:257:PRO:CD	2.83	0.42
1:B:263:ALA:HB3	1:B:336:ALA:HB1	2.02	0.42
3:S:144:TRP:HB3	3:S:145:PRO:HD2	2.00	0.42
1:A:243:ALA:O	1:A:247:VAL:HG23	2.19	0.42
1:C:226:VAL:HG11	2:R:223:ARG:CZ	2.50	0.42
1:C:99:GLU:O	1:C:100:GLY:C	2.56	0.42
1:A:28:ARG:HE	1:A:28:ARG:HB2	1.69	0.41
1:C:133:TYR:CE2	1:C:135:VAL:CG2	3.03	0.41
1:C:286:LYS:HD3	1:C:291:HIS:CE1	2.55	0.41
1:C:310:MET:HA	1:C:313:GLN:NE2	2.34	0.41
1:C:330:SER:HB3	1:C:386:VAL:HG23	2.01	0.41
2:R:240:GLN:HG3	2:R:327:THR:HG23	2.02	0.41
1:B:171:GLY:HA3	1:B:223:ARG:HD3	2.02	0.41
1:C:370:LYS:HD3	1:D:345:THR:HG22	2.01	0.41
1:D:29:LYS:HG2	3:S:192:TYR:CE1	2.55	0.41
1:B:324:ARG:NH2	1:B:389:GLU:OE1	2.53	0.41
1:D:134:CYS:HA	1:D:167:ILE:HD12	2.02	0.41
1:A:123:ARG:CG	1:A:124:MET:HE3	2.51	0.41
1:B:99:GLU:O	1:B:100:GLY:C	2.59	0.41
2:R:225:LEU:CD1	2:R:234:LEU:HD11	2.50	0.41
1:D:166:TRP:O	4:D:3399:FAD:C4X	2.69	0.41
1:A:122:GLY:O	1:A:125:THR:HB	2.20	0.41
1:B:275:THR:HG21	1:C:394:TYR:CD1	2.55	0.41
1:D:341:ASN:OD1	1:D:370:LYS:HA	2.21	0.41
2:R:301:LYS:HG2	4:R:599:FAD:N3A	2.36	0.41
3:S:148:THR:OG1	3:S:164:ARG:NH2	2.53	0.41
1:B:289:VAL:HG22	1:C:391:ILE:HD13	2.03	0.41
1:D:267:ALA:HB1	1:D:343:LEU:HD22	2.03	0.41
1:A:363:GLU:OE2	1:A:367:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:CG	1:B:256:ARG:NH1	2.81	0.41
1:B:330:SER:OG	1:B:385:ILE:HG21	2.21	0.41
3:S:122:LEU:HD23	5:S:600:AMP:H1'	2.02	0.41
1:A:377:GLY:HA2	6:A:412:HOH:O	2.20	0.41
1:B:36:ILE:HG13	1:B:90:GLY:HA2	2.03	0.41
1:C:166:TRP:O	4:C:2399:FAD:N5	2.54	0.41
1:C:195:THR:HG23	6:C:2412:HOH:O	2.20	0.41
1:D:178:LEU:O	1:D:196:GLY:HA2	2.21	0.41
1:D:253:ASP:CA	1:D:325:ASN:HD21	2.33	0.41
2:R:219:VAL:HG22	2:R:276:ILE:HD12	2.03	0.41
1:B:106:MET:HE2	1:B:254:LYS:HD3	2.03	0.40
1:B:244:GLY:O	1:B:247:VAL:HG22	2.21	0.40
1:C:305:VAL:HG23	1:C:343:LEU:HD21	2.02	0.40
4:C:2399:FAD:H8A	1:D:283:THR:HG21	2.03	0.40
1:D:123:ARG:HD3	1:D:174:ASN:HD21	1.86	0.40
3:S:14:ILE:O	3:S:15:ASP:C	2.59	0.40
1:A:298:LEU:HD23	1:D:391:ILE:HD11	2.03	0.40
1:D:259:VAL:HG21	1:D:376:GLU:CG	2.44	0.40
2:R:223:ARG:NH2	2:R:250:ALA:HB1	2.36	0.40
2:R:264:GLY:HA2	2:R:289:GLY:HA3	2.04	0.40
1:B:108:ILE:HD11	1:B:198:ILE:HG12	2.04	0.40
1:D:85:GLU:HG3	1:D:264:VAL:HG22	2.02	0.40
3:S:15:ASP:HB3	3:S:18:VAL:HG23	2.04	0.40
3:S:38:MET:O	3:S:39:ASN:C	2.59	0.40
1:B:91:CYS:SG	1:B:94:VAL:HG13	2.62	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	384/421 (91%)	361 (94%)	22 (6%)	1 (0%)	41 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	385/421 (91%)	368 (96%)	15 (4%)	2 (0%)	29	61
1	C	386/421 (92%)	372 (96%)	12 (3%)	2 (0%)	29	61
1	D	385/421 (91%)	365 (95%)	20 (5%)	0	100	100
2	R	309/333 (93%)	270 (87%)	31 (10%)	8 (3%)	5	18
3	S	235/255 (92%)	205 (87%)	25 (11%)	5 (2%)	7	23
All	All	2084/2272 (92%)	1941 (93%)	125 (6%)	18 (1%)	17	46

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	C	234	LYS
3	S	218	LEU
2	R	30	ASN
2	R	50	GLU
2	R	242	HIS
3	S	217	ASP
2	R	306	PRO
3	S	94	ALA
1	B	191	ASN
2	R	48	GLY
2	R	60	CYS
3	S	25	ASP
2	R	290	MET
1	B	141	GLY
2	R	36	ILE
3	S	177	LEU
1	C	141	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/332 (86%)	259 (90%)	28 (10%)	8	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	288/332 (87%)	260 (90%)	28 (10%)	8	24
1	C	293/332 (88%)	257 (88%)	36 (12%)	4	15
1	D	296/332 (89%)	263 (89%)	33 (11%)	6	19
2	R	232/262 (88%)	204 (88%)	28 (12%)	5	15
3	S	183/213 (86%)	163 (89%)	20 (11%)	6	19
All	All	1579/1803 (88%)	1406 (89%)	173 (11%)	6	19

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	59	LEU
1	A	61	LEU
1	A	68	GLU
1	A	73	LEU
1	A	82	LEU
1	A	118	LYS
1	A	130	MET
1	A	154	LYS
1	A	172	LYS
1	A	191	ASN
1	A	210	ARG
1	A	218	ARG
1	A	225	ILE
1	A	226	VAL
1	A	235	GLU
1	A	249	MET
1	A	266	LEU
1	A	276	LYS
1	A	289	VAL
1	A	298	LEU
1	A	307	LEU
1	A	312	TYR
1	A	323	ARG
1	A	339	ILE
1	A	375	TYR
1	A	383	ARG
1	A	395	LYS
1	B	32	ARG
1	B	47	GLU

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Mol	Chain	Res	Type
1	B	55	ARG
1	B	95	GLN
1	B	117	LYS
1	B	121	LEU
1	B	125	THR
1	B	127	GLU
1	B	152	GLU
1	B	156	ASP
1	B	182	SER
1	B	207	GLN
1	B	210	ARG
1	B	218	ARG
1	B	223	ARG
1	B	228	GLU
1	B	235	GLU
1	B	239	ILE
1	B	256	ARG
1	B	289	VAL
1	B	295	SER
1	B	312	TYR
1	B	345	THR
1	B	371	ILE
1	B	375	TYR
1	B	379	SER
1	B	392	ASP
1	B	393	LYS
1	C	10	LEU
1	C	19	GLN
1	C	47	GLU
1	C	54	ARG
1	C	75	LEU
1	C	92	THR
1	C	103	LEU
1	C	114	ASP
1	C	129	LEU
1	C	150	LYS
1	C	163	GLN
1	C	165	MET
1	C	179	LEU
1	C	182	SER
1	C	210	ARG
1	C	213	LEU

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Mol	Chain	Res	Type
1	C	221	ASP
1	C	222	THR
1	C	226	VAL
1	C	237	VAL
1	C	238	LEU
1	C	241	ASP
1	C	249	MET
1	C	256	ARG
1	C	259	VAL
1	C	266	LEU
1	C	286	LYS
1	C	298	LEU
1	C	307	LEU
1	C	311	SER
1	C	312	TYR
1	C	358	THR
1	C	359	GLU
1	C	363	GLU
1	C	375	TYR
1	C	379	SER
1	D	15	GLU
1	D	33	GLU
1	D	63	ASN
1	D	75	LEU
1	D	94	VAL
1	D	95	GLN
1	D	98	ILE
1	D	115	GLN
1	D	134	CYS
1	D	172	LYS
1	D	178	LEU
1	D	192	LYS
1	D	210	ARG
1	D	219	CYS
1	D	234	LYS
1	D	235	GLU
1	D	238	LEU
1	D	241	ASP
1	D	264	VAL
1	D	266	LEU
1	D	269	ARG
1	D	282	LYS

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Mol	Chain	Res	Type
1	D	324	ARG
1	D	325	ASN
1	D	339	ILE
1	D	343	LEU
1	D	345	THR
1	D	358	THR
1	D	359	GLU
1	D	375	TYR
1	D	379	SER
1	D	381	ILE
1	D	392	ASP
2	R	20	GLN
2	R	30	ASN
2	R	52	SER
2	R	53	CYS
2	R	58	THR
2	R	95	LEU
2	R	104	ASN
2	R	106	THR
2	R	118	ASN
2	R	126	LYS
2	R	147	THR
2	R	159	CYS
2	R	163	VAL
2	R	174	ASP
2	R	178	THR
2	R	190	SER
2	R	198	GLU
2	R	205	THR
2	R	209	ARG
2	R	225	LEU
2	R	261	MET
2	R	273	GLU
2	R	285	GLN
2	R	295	THR
2	R	310	VAL
2	R	312	ASP
2	R	330	LEU
2	R	332	LYS
3	S	20	ILE
3	S	22	VAL
3	S	37	SER

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Mol	Chain	Res	Type
3	S	70	GLN
3	S	76	ARG
3	S	85	ARG
3	S	111	LEU
3	S	149	PHE
3	S	154	THR
3	S	155	LEU
3	S	164	ARG
3	S	177	LEU
3	S	185	LEU
3	S	188	ASN
3	S	194	THR
3	S	219	THR
3	S	226	SER
3	S	241	THR
3	S	242	THR
3	S	244	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	101	ASN
1	A	105	GLN
1	A	161	ASN
1	A	169	ASN
1	A	191	ASN
1	A	341	ASN
1	A	349	GLN
1	A	373	GLN
1	A	380	GLN
1	B	65	HIS
1	B	95	GLN
1	B	161	ASN
1	B	163	GLN
1	B	349	GLN
1	B	380	GLN
1	B	382	GLN
1	C	161	ASN
1	C	313	GLN
1	C	349	GLN
1	C	373	GLN

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Mol	Chain	Res	Type
1	C	382	GLN
1	D	19	GLN
1	D	69	ASN
1	D	115	GLN
1	D	163	GLN
1	D	174	ASN
1	D	236	ASN
1	D	325	ASN
1	D	354	ASN
1	D	373	GLN
2	R	30	ASN
2	R	39	ASN
2	R	118	ASN
2	R	262	GLN
2	R	285	GLN
3	S	39	ASN
3	S	70	GLN
3	S	146	GLN
3	S	188	ASN
3	S	197	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FAD	C	2399	-	51,58,58	1.52	8 (15%)	60,89,89	1.81	10 (16%)
4	FAD	A	399	-	51,58,58	1.31	7 (13%)	60,89,89	1.92	14 (23%)
4	FAD	D	3399	-	51,58,58	1.39	7 (13%)	60,89,89	1.89	11 (18%)
5	AMP	S	600	-	22,25,25	0.95	1 (4%)	25,38,38	1.56	6 (24%)
4	FAD	B	1399	-	51,58,58	1.41	7 (13%)	60,89,89	1.79	9 (15%)
4	FAD	R	599	-	51,58,58	1.42	6 (11%)	60,89,89	1.84	10 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	C	2399	-	-	2/30/50/50	0/6/6/6
4	FAD	A	399	-	-	6/30/50/50	0/6/6/6
4	FAD	D	3399	-	-	0/30/50/50	0/6/6/6
5	AMP	S	600	-	-	3/6/26/26	0/3/3/3
4	FAD	B	1399	-	-	2/30/50/50	0/6/6/6
4	FAD	R	599	-	-	11/30/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	599	FAD	C10-N1	4.82	1.39	1.33
4	R	599	FAD	C2A-N3A	4.11	1.38	1.32
4	A	399	FAD	C2A-N3A	4.06	1.38	1.32
4	C	2399	FAD	C10-N1	4.03	1.38	1.33
4	C	2399	FAD	C4-N3	3.95	1.39	1.33
4	B	1399	FAD	C2A-N3A	3.81	1.38	1.32
4	D	3399	FAD	C10-N1	3.76	1.38	1.33
4	C	2399	FAD	C4X-N5	3.71	1.38	1.33
4	C	2399	FAD	C1'-N10	3.63	1.52	1.48
4	R	599	FAD	C4X-N5	3.58	1.38	1.33
4	D	3399	FAD	C2A-N3A	3.50	1.37	1.32
4	D	3399	FAD	C4X-N5	3.49	1.38	1.33
4	B	1399	FAD	C1'-N10	3.46	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1399	FAD	C4-N3	3.41	1.39	1.33
4	B	1399	FAD	C4X-N5	3.33	1.38	1.33
4	A	399	FAD	C10-N1	3.31	1.37	1.33
4	D	3399	FAD	C1'-N10	3.28	1.51	1.48
4	B	1399	FAD	C10-N1	3.27	1.37	1.33
4	R	599	FAD	C4-N3	3.20	1.38	1.33
4	A	399	FAD	C4X-N5	3.14	1.37	1.33
4	C	2399	FAD	C2A-N3A	3.12	1.37	1.32
4	R	599	FAD	C2A-N1A	2.95	1.39	1.33
4	D	3399	FAD	C4-N3	2.94	1.38	1.33
4	A	399	FAD	C1'-N10	2.85	1.51	1.48
4	C	2399	FAD	C2A-N1A	2.78	1.39	1.33
4	D	3399	FAD	C2A-N1A	2.76	1.39	1.33
4	A	399	FAD	C2A-N1A	2.41	1.38	1.33
4	B	1399	FAD	C5X-N5	2.29	1.39	1.35
4	B	1399	FAD	C2A-N1A	2.24	1.38	1.33
4	A	399	FAD	C5X-N5	2.24	1.39	1.35
4	A	399	FAD	C4-N3	2.23	1.36	1.33
5	S	600	AMP	C5-C4	2.10	1.46	1.40
4	R	599	FAD	C1'-N10	2.10	1.50	1.48
4	D	3399	FAD	O4B-C4B	-2.04	1.40	1.45
4	C	2399	FAD	C2B-C1B	-2.02	1.50	1.53
4	C	2399	FAD	O4'-C4'	-2.01	1.39	1.43

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3399	FAD	C4-N3-C2	7.78	121.71	115.14
4	C	2399	FAD	C4-N3-C2	6.92	120.98	115.14
4	R	599	FAD	N3A-C2A-N1A	-6.34	118.77	128.68
4	B	1399	FAD	C4-N3-C2	6.25	120.42	115.14
4	A	399	FAD	N3A-C2A-N1A	-5.98	119.34	128.68
4	R	599	FAD	C4-N3-C2	5.81	120.05	115.14
4	B	1399	FAD	N3A-C2A-N1A	-5.62	119.90	128.68
4	D	3399	FAD	N3A-C2A-N1A	-5.51	120.06	128.68
4	B	1399	FAD	C1'-N10-C9A	5.41	122.55	118.29
4	A	399	FAD	C4-N3-C2	5.30	119.61	115.14
4	A	399	FAD	C5X-C9A-N10	5.04	121.37	117.72
4	C	2399	FAD	N3A-C2A-N1A	-5.03	120.81	128.68
4	R	599	FAD	C4X-N5-C5X	4.80	121.57	116.77
4	A	399	FAD	C5A-C6A-N6A	-4.55	113.44	120.35
4	R	599	FAD	C1'-N10-C9A	4.48	121.82	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3399	FAD	C5X-C9A-N10	4.28	120.82	117.72
4	D	3399	FAD	C4X-C4-N3	-4.17	117.72	123.43
4	C	2399	FAD	C4X-C4-N3	-4.05	117.89	123.43
4	A	399	FAD	C1'-N10-C9A	3.93	121.39	118.29
4	C	2399	FAD	C1'-N10-C9A	3.89	121.35	118.29
4	C	2399	FAD	O5'-C5'-C4'	-3.82	99.16	109.36
4	A	399	FAD	C4X-N5-C5X	3.72	120.49	116.77
4	D	3399	FAD	C4X-N5-C5X	3.60	120.37	116.77
4	D	3399	FAD	P-O3P-PA	-3.27	121.59	132.83
4	R	599	FAD	C10-C4X-N5	-3.26	119.00	121.26
4	B	1399	FAD	C4X-C4-N3	-3.24	119.00	123.43
4	B	1399	FAD	C4X-N5-C5X	3.23	120.00	116.77
4	D	3399	FAD	C1'-N10-C10	3.22	121.29	118.41
5	S	600	AMP	N3-C2-N1	-3.14	123.78	128.68
4	A	399	FAD	C4X-C4-N3	-3.12	119.17	123.43
4	C	2399	FAD	P-O3P-PA	-3.10	122.17	132.83
5	S	600	AMP	O2P-P-O5'	-3.06	98.58	106.73
5	S	600	AMP	C4-C5-N7	-3.06	106.21	109.40
4	C	2399	FAD	C5X-C9A-N10	3.00	119.89	117.72
4	R	599	FAD	P-O3P-PA	-2.94	122.75	132.83
4	B	1399	FAD	C5X-C9A-N10	2.93	119.84	117.72
4	R	599	FAD	O4'-C4'-C3'	2.93	116.22	109.10
4	A	399	FAD	C9A-N10-C10	-2.86	118.16	121.91
4	B	1399	FAD	P-O3P-PA	-2.85	123.04	132.83
4	B	1399	FAD	C10-C4X-N5	-2.76	119.35	121.26
4	A	399	FAD	C8M-C8-C9	-2.69	113.92	120.34
4	B	1399	FAD	C9A-N10-C10	-2.68	118.40	121.91
5	S	600	AMP	C2-N1-C6	2.56	123.13	118.75
4	C	2399	FAD	C4X-N5-C5X	2.52	119.28	116.77
4	C	2399	FAD	C10-C4X-N5	-2.47	119.55	121.26
4	D	3399	FAD	C1B-N9A-C4A	-2.46	122.31	126.64
4	A	399	FAD	C10-C4X-N5	-2.41	119.59	121.26
4	R	599	FAD	C2A-N1A-C6A	2.38	122.83	118.75
4	R	599	FAD	C4-C4X-N5	2.36	121.29	118.60
5	S	600	AMP	O3P-P-O2P	2.30	116.42	107.64
4	A	399	FAD	C1'-N10-C10	2.28	120.45	118.41
4	A	399	FAD	P-O3P-PA	-2.24	125.13	132.83
4	A	399	FAD	C8M-C8-C7	2.21	125.28	120.74
4	R	599	FAD	C4X-C4-N3	-2.17	120.47	123.43
4	D	3399	FAD	C10-C4X-N5	-2.13	119.79	121.26
4	C	2399	FAD	O2P-P-O5'	2.08	117.42	107.75
4	D	3399	FAD	C8M-C8-C9	-2.06	115.41	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3399	FAD	C8M-C8-C7	2.02	124.88	120.74
4	A	399	FAD	C9A-C5X-N5	-2.02	119.21	122.36
5	S	600	AMP	C5-C6-N1	-2.00	115.81	120.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	399	FAD	C2'-C1'-N10-C10
4	C	2399	FAD	C3'-C4'-C5'-O5'
4	C	2399	FAD	O4'-C4'-C5'-O5'
4	R	599	FAD	O4B-C4B-C5B-O5B
4	R	599	FAD	C1'-C2'-C3'-C4'
4	R	599	FAD	C3'-C4'-C5'-O5'
4	R	599	FAD	O4'-C4'-C5'-O5'
4	R	599	FAD	C3B-C4B-C5B-O5B
5	S	600	AMP	O4'-C4'-C5'-O5'
5	S	600	AMP	C3'-C4'-C5'-O5'
4	R	599	FAD	O2'-C2'-C3'-O3'
4	R	599	FAD	O2'-C2'-C3'-C4'
4	A	399	FAD	O2'-C2'-C3'-C4'
4	B	1399	FAD	PA-O3P-P-O1P
4	A	399	FAD	O2'-C2'-C3'-O3'
4	A	399	FAD	C5B-O5B-PA-O3P
4	R	599	FAD	C5B-O5B-PA-O3P
4	A	399	FAD	C5B-O5B-PA-O1A
4	A	399	FAD	C1'-C2'-C3'-O3'
4	R	599	FAD	C1'-C2'-C3'-O3'
5	S	600	AMP	C5'-O5'-P-O1P
4	B	1399	FAD	PA-O3P-P-O2P
4	R	599	FAD	C5B-O5B-PA-O1A
4	R	599	FAD	N10-C1'-C2'-O2'

There are no ring outliers.

6 monomers are involved in 24 short contacts:

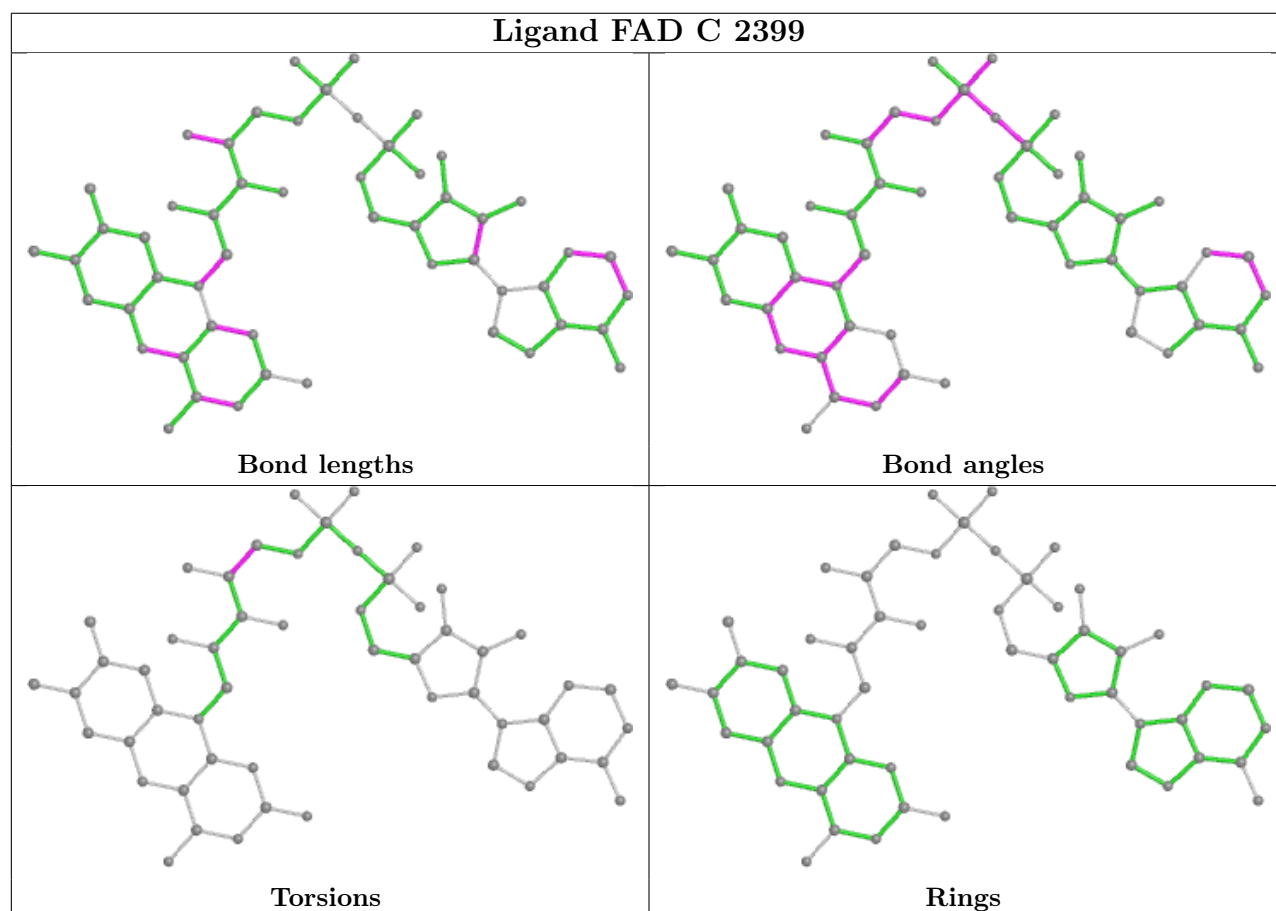
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2399	FAD	5	0
4	A	399	FAD	7	0
4	D	3399	FAD	4	0
5	S	600	AMP	1	0

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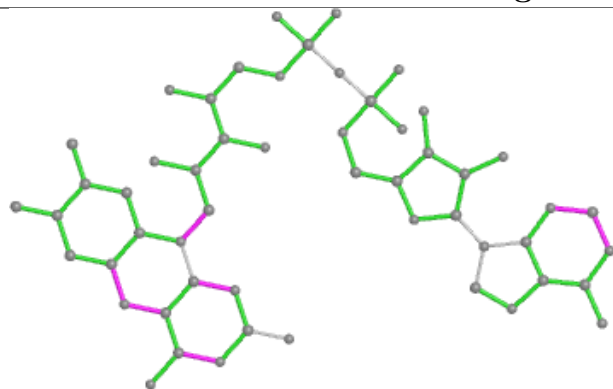
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1399	FAD	3	0
4	R	599	FAD	4	0

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.

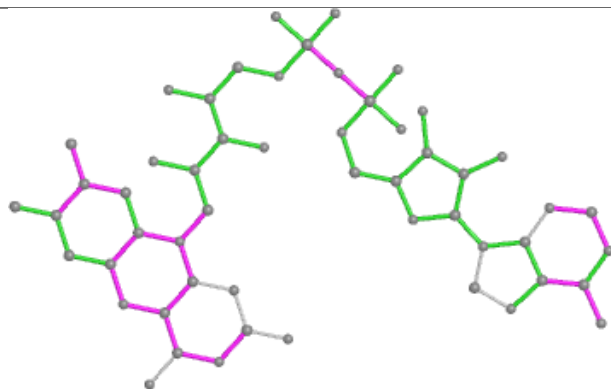




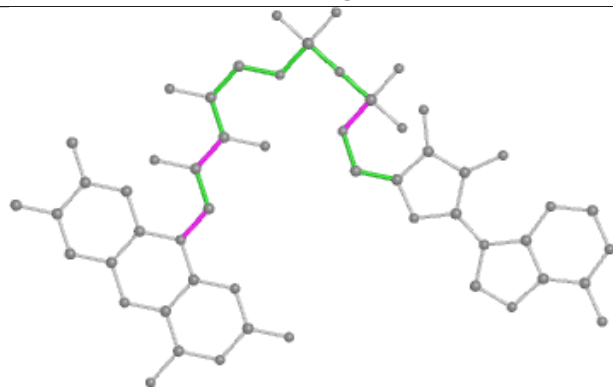
## Ligand FAD A 399



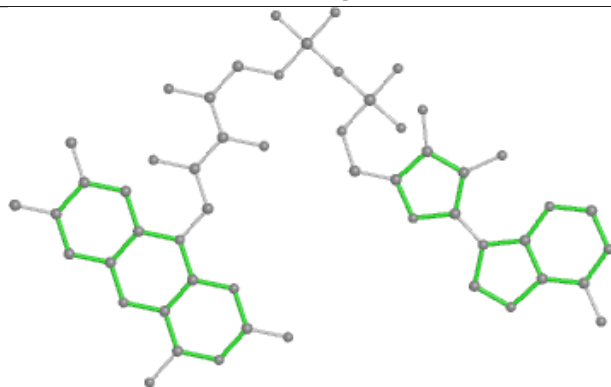
Bond lengths



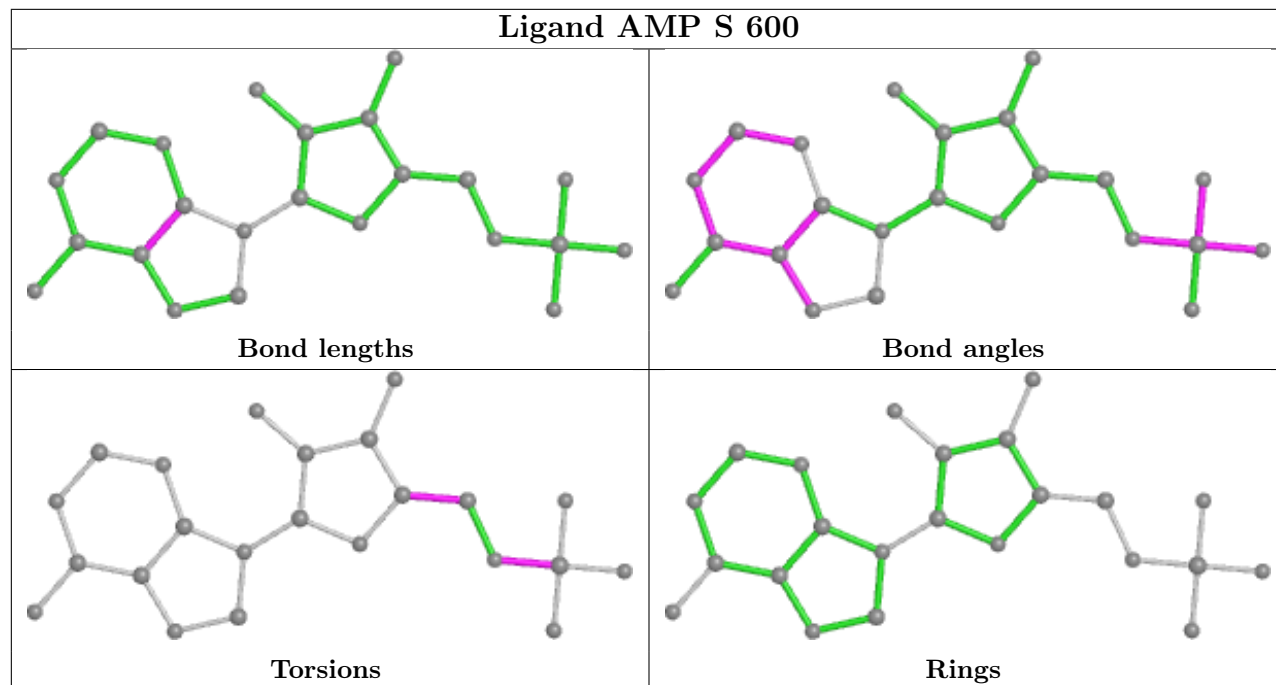
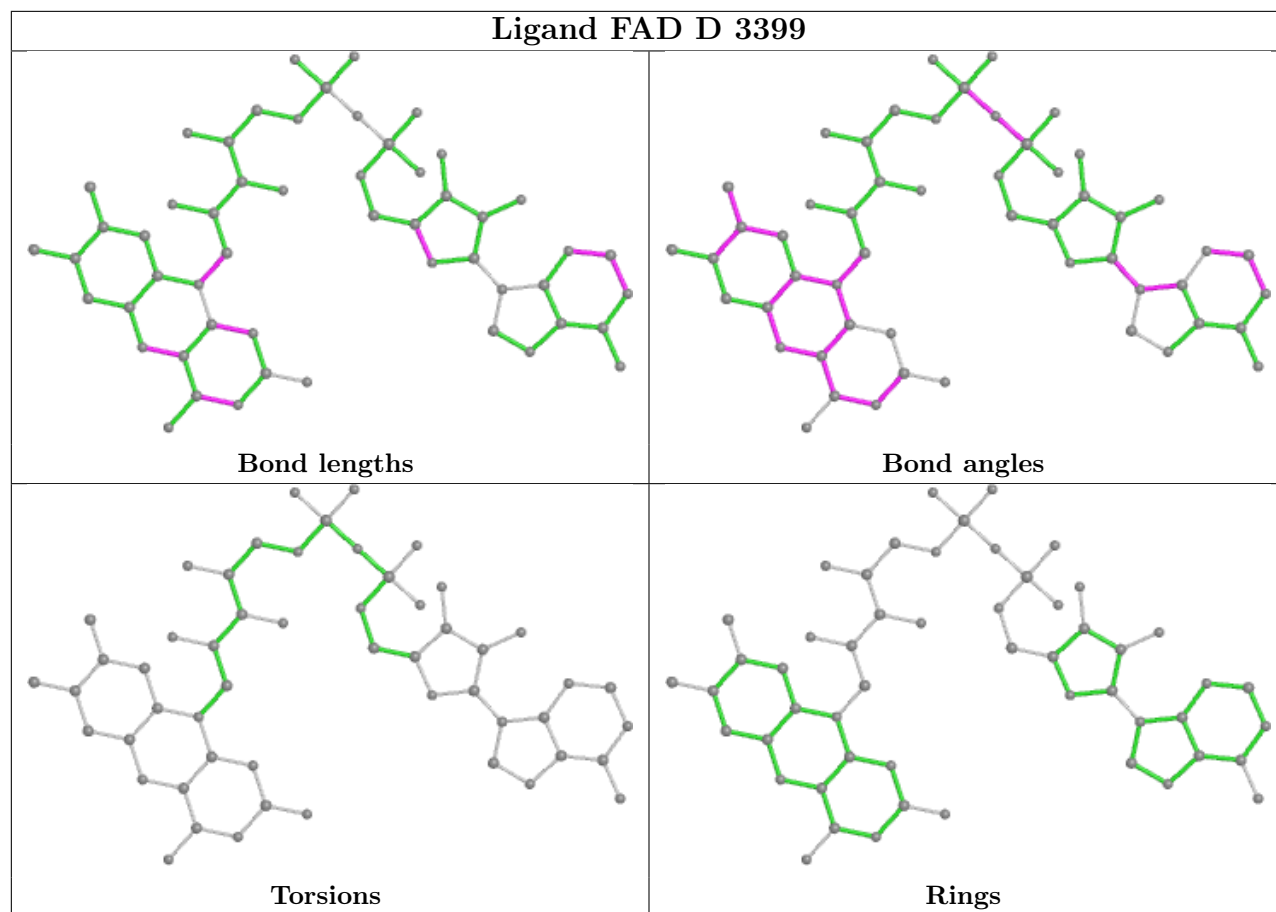
Bond angles

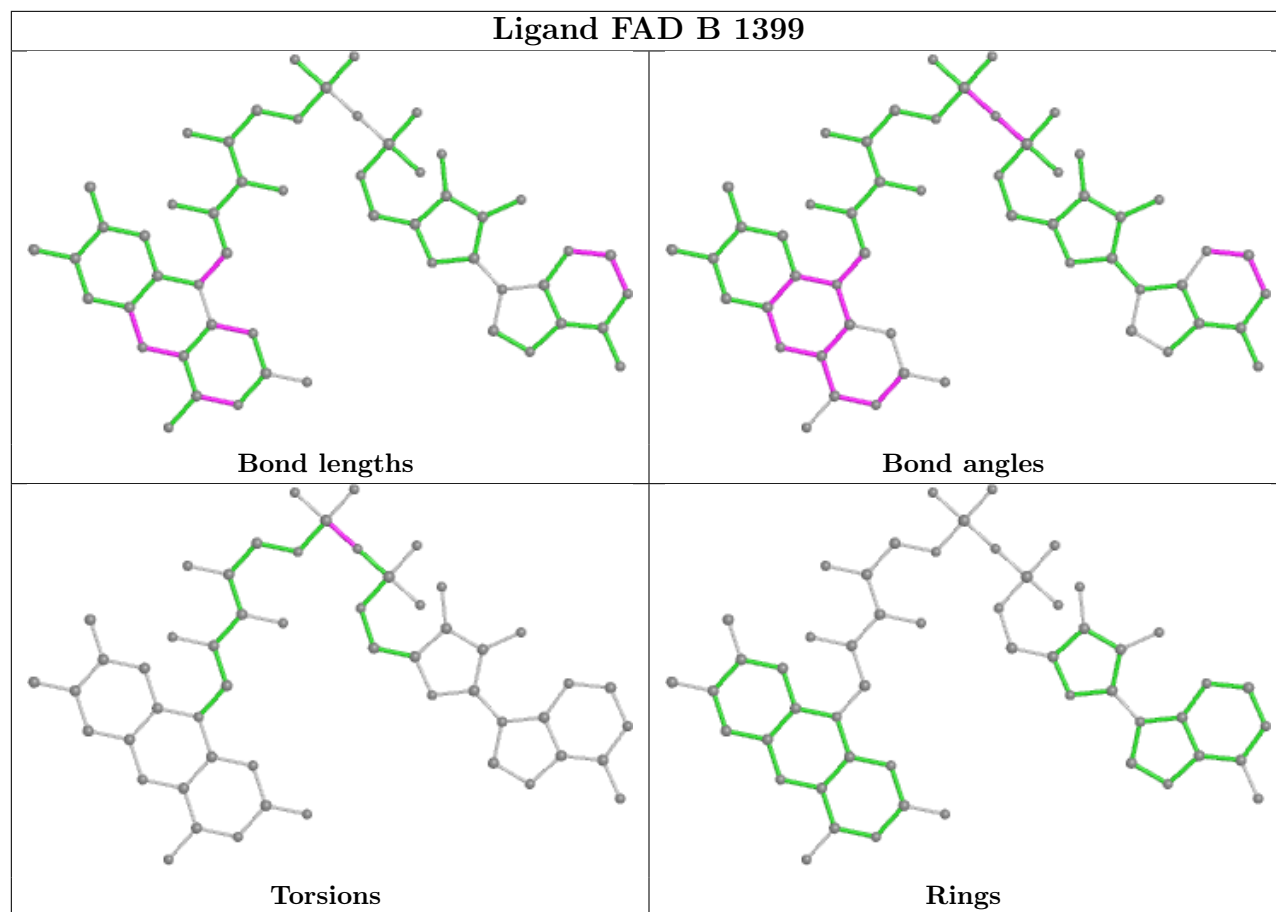


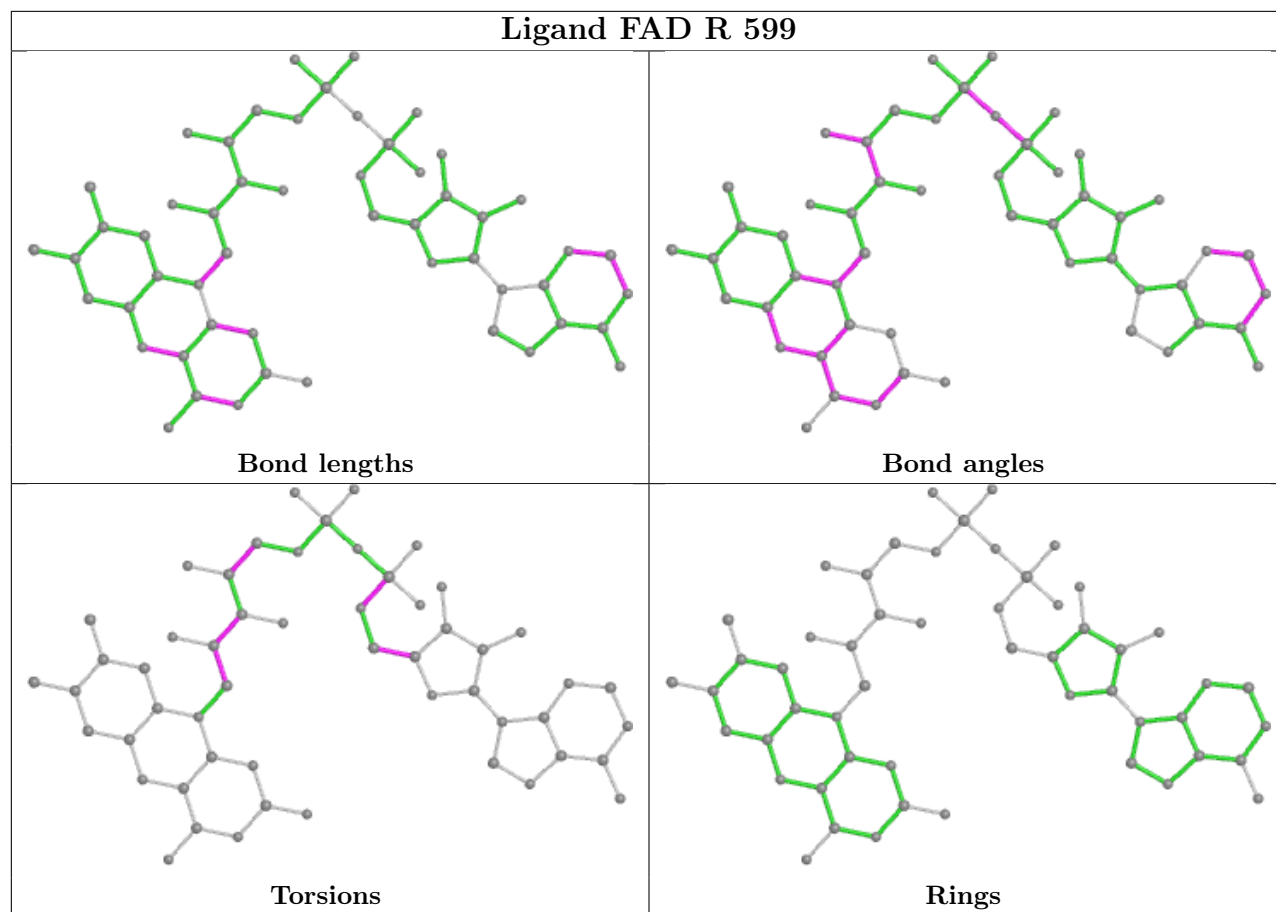
Torsions



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	386/421 (91%)	-0.53	1 (0%) 94 93	26, 37, 49, 57	0
1	B	387/421 (91%)	-0.45	2 (0%) 91 88	26, 40, 53, 62	0
1	C	388/421 (92%)	-0.56	1 (0%) 94 93	24, 37, 49, 60	0
1	D	387/421 (91%)	-0.52	3 (0%) 86 81	24, 37, 51, 60	0
2	R	313/333 (93%)	0.56	40 (12%) 3 2	43, 63, 91, 104	0
3	S	239/255 (93%)	0.04	10 (4%) 36 26	36, 53, 77, 111	0
All	All	2100/2272 (92%)	-0.29	57 (2%) 54 44	24, 41, 82, 111	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	333	LYS	6.2
2	R	220	SER	5.0
2	R	213	THR	4.8
2	R	303	PRO	4.7
2	R	242	HIS	4.6
2	R	209	ARG	4.5
2	R	332	LYS	4.1
2	R	221	GLY	3.9
3	S	247	ALA	3.8
3	S	241	THR	3.8
2	R	227	SER	3.6
2	R	19	PHE	3.4
2	R	253	ASP	3.3
3	S	246	VAL	3.2
2	R	18	ARG	3.2
2	R	210	PRO	3.1
3	S	24	PRO	3.0
2	R	248	SER	3.0
1	B	396	ASN	3.0

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	C	396	ASN	3.0
2	R	277	ALA	2.8
2	R	276	ILE	2.8
3	S	33	GLY	2.8
2	R	255	GLY	2.7
2	R	292	ASP	2.6
1	D	10	LEU	2.6
2	R	316	VAL	2.6
1	D	156	ASP	2.5
2	R	232	LYS	2.5
2	R	240	GLN	2.4
2	R	331	LYS	2.4
2	R	174	ASP	2.4
2	R	296	ILE	2.4
2	R	310	VAL	2.4
3	S	243	GLU	2.4
2	R	182	SER	2.4
2	R	254	ALA	2.4
3	S	25	ASP	2.3
1	D	396	ASN	2.3
3	S	242	THR	2.3
2	R	175	ALA	2.3
2	R	23	LEU	2.2
2	R	229	GLU	2.2
2	R	171	THR	2.1
2	R	269	ILE	2.1
3	S	250	LYS	2.1
2	R	312	ASP	2.1
1	B	69	ASN	2.1
3	S	248	LYS	2.1
2	R	214	GLY	2.0
2	R	211	GLU	2.0
2	R	258	PRO	2.0
2	R	278	VAL	2.0
2	R	238	ALA	2.0
2	R	317	ALA	2.0
1	A	186	PRO	2.0
2	R	260	ASP	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 [i](#)

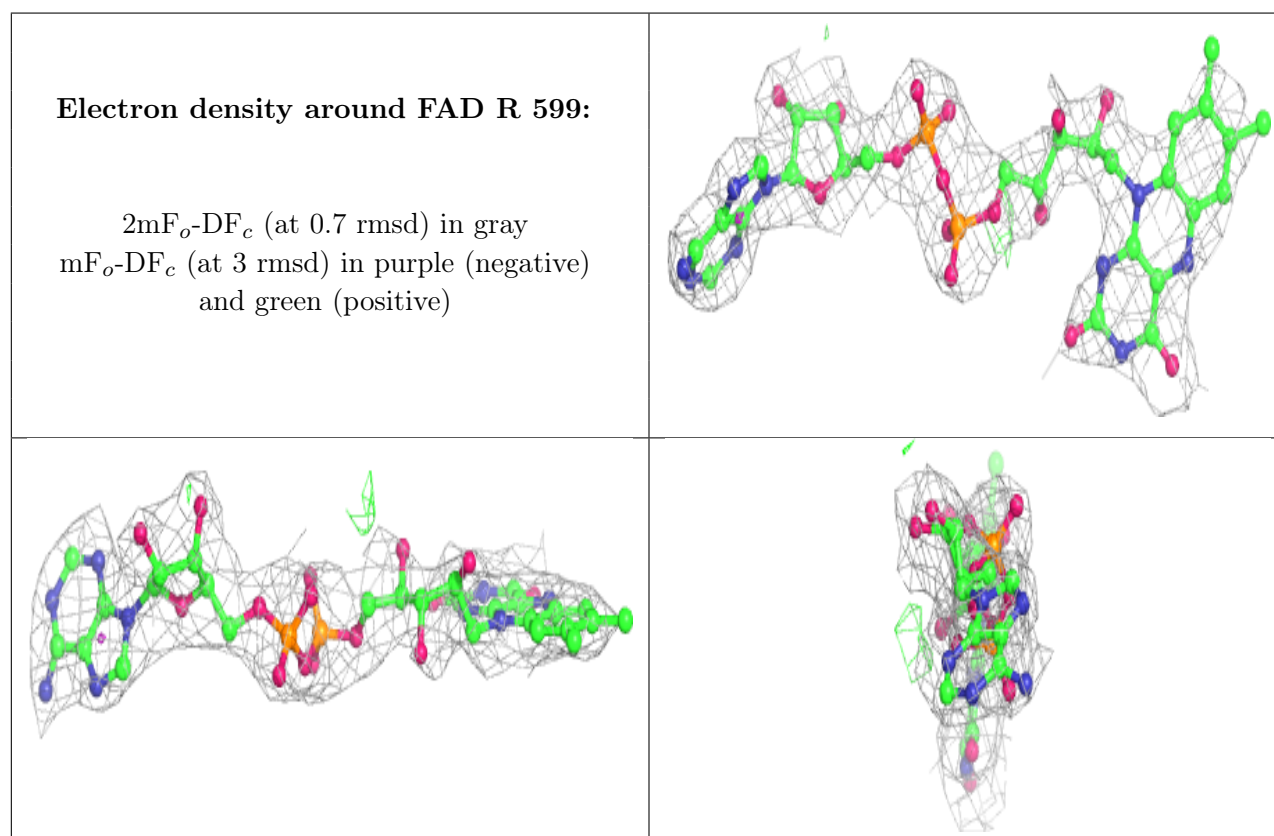
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

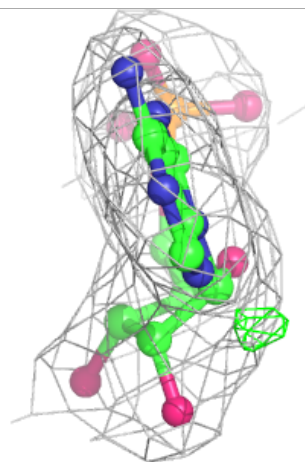
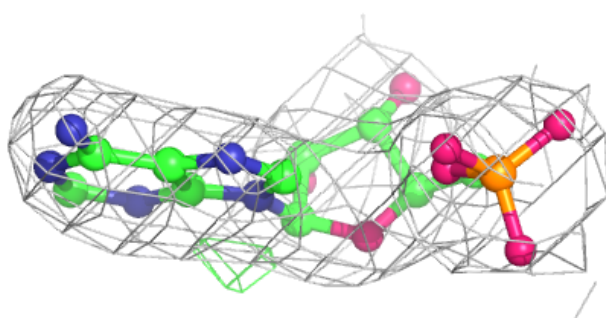
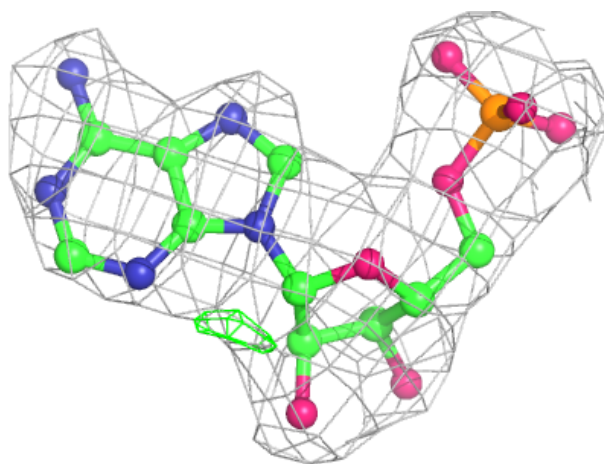
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FAD	R	599	53/53	0.91	0.17	61,65,71,71	0
5	AMP	S	600	23/23	0.96	0.12	41,45,46,46	0
4	FAD	C	2399	53/53	0.97	0.12	29,33,36,37	0
4	FAD	D	3399	53/53	0.97	0.11	28,32,37,37	0
4	FAD	A	399	53/53	0.97	0.12	27,33,35,36	0
4	FAD	B	1399	53/53	0.97	0.13	29,35,41,42	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 AMP S 600:**

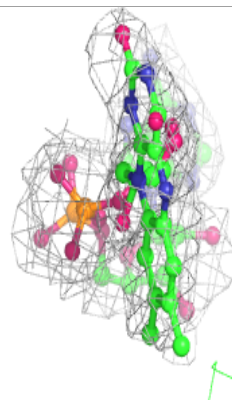
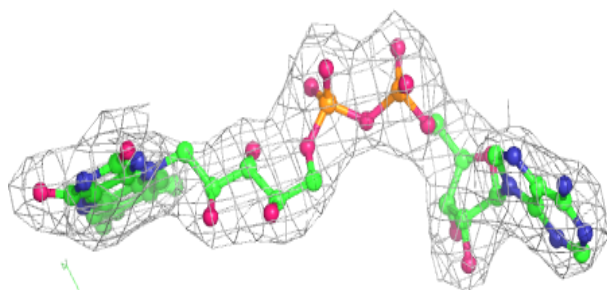
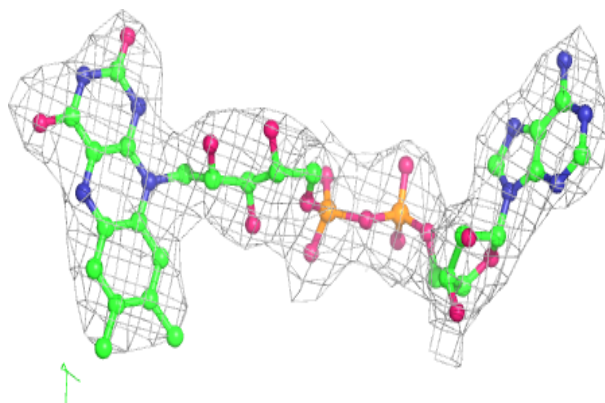
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



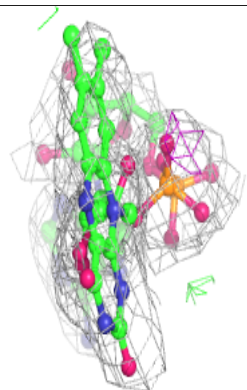
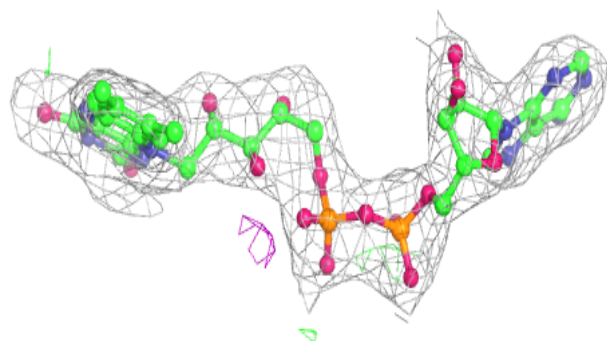
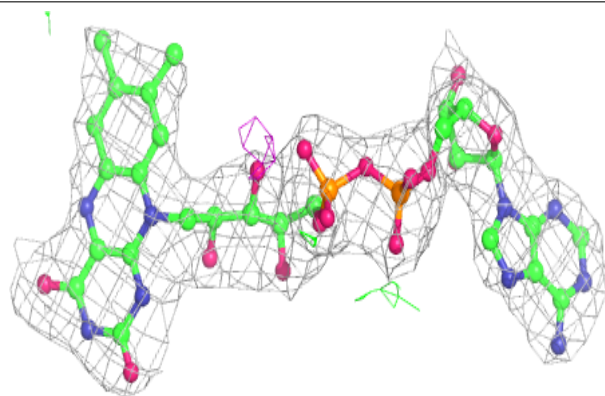


**Electron density around FAD C 2399:**

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

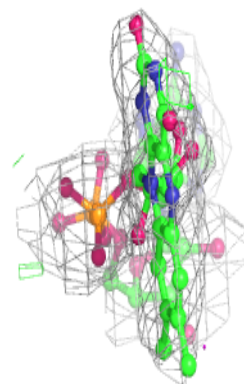
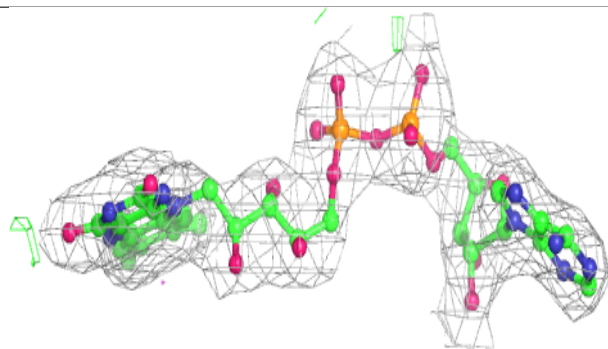
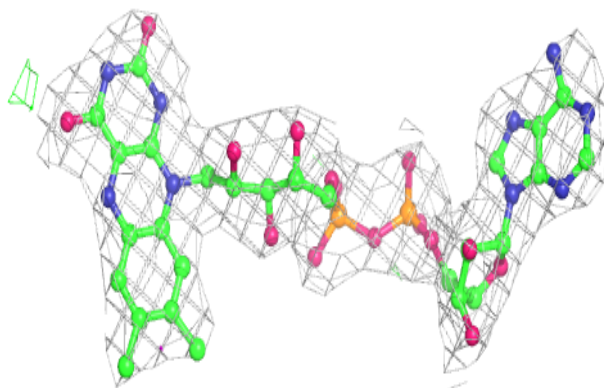
**Electron density around FAD D 3399:**

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

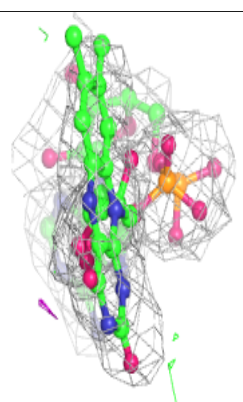
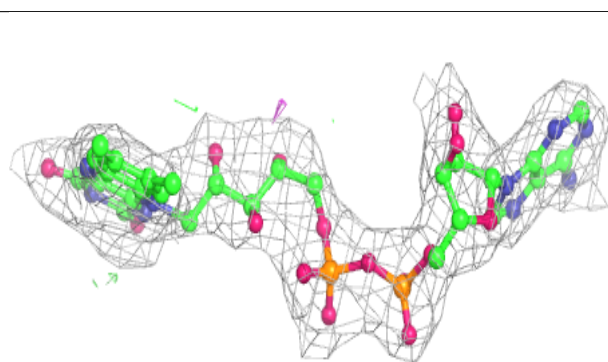
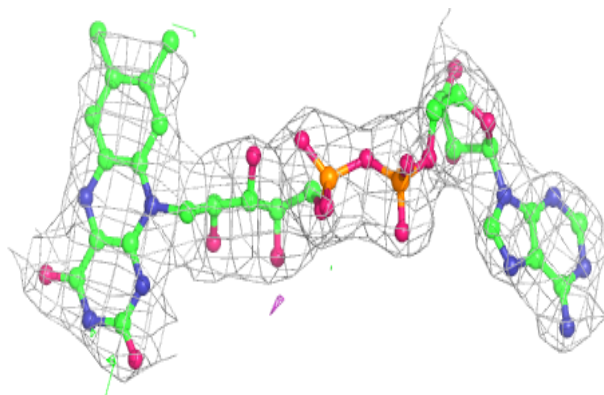


**Electron density around FAD A 399:**

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

**Electron density around FAD B 1399:**

$2mF_o-DF_c$  (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.