



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:24 AM GMT

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 wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

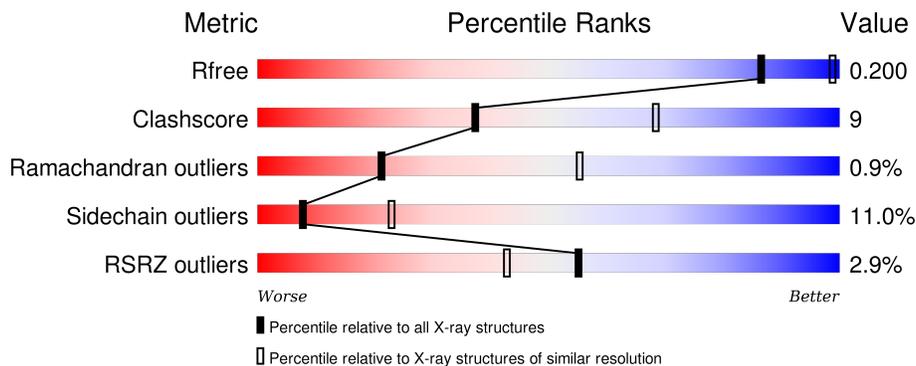
# 1 Overall quality at a glance i

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	 68% 21% • 8%
1	B	421	 69% 21% • 8%
1	C	421	 72% 18% • 8%
1	D	421	 68% 20% • 8%
2	R	333	 13% 67% 23% • 6%

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Mol	Chain	Length	Quality of chain
3	S	255	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '4%', a large green segment labeled '68%', a yellow segment labeled '22%', and a small grey segment at the end labeled '6%'.</p>

## 2 Entry composition [i](#)

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 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).



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

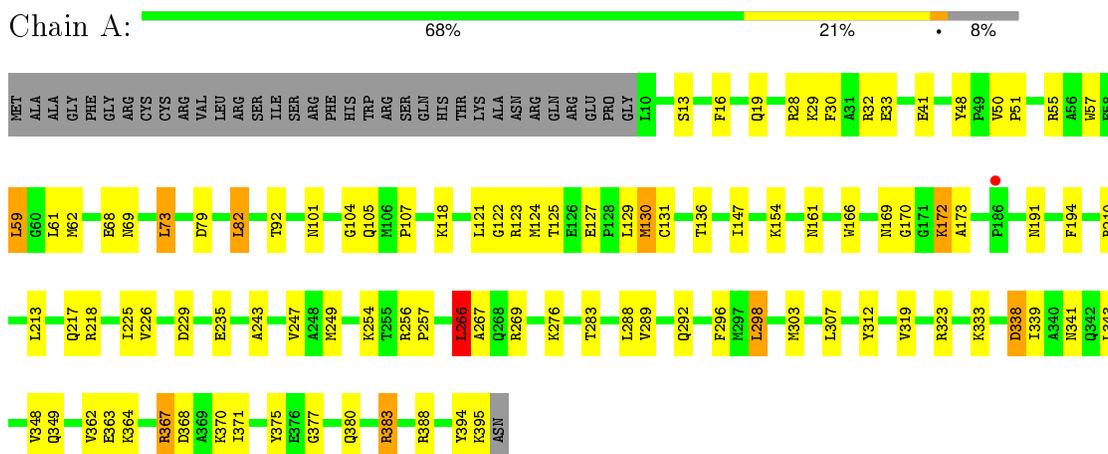
- Molecule 6 is water.

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		

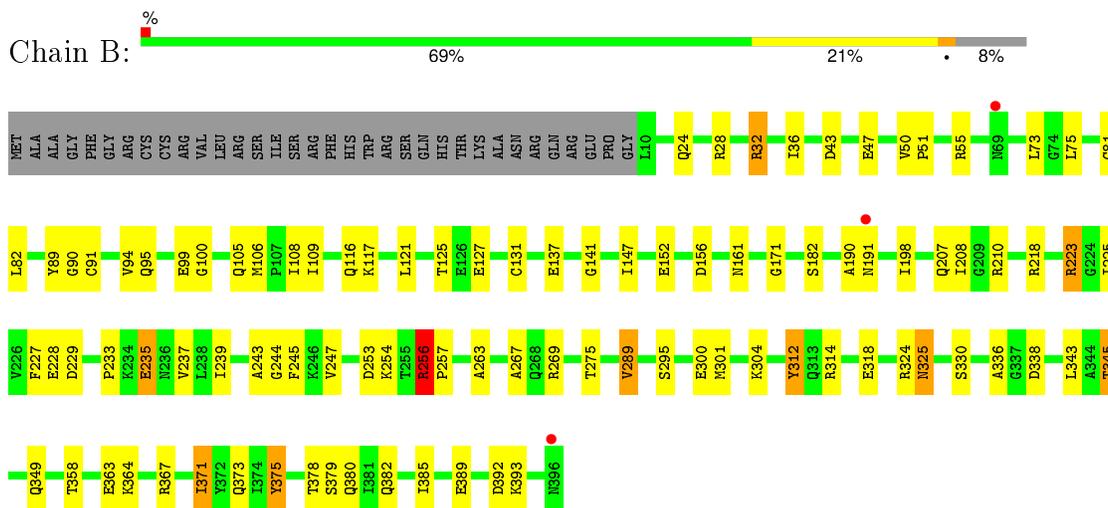
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

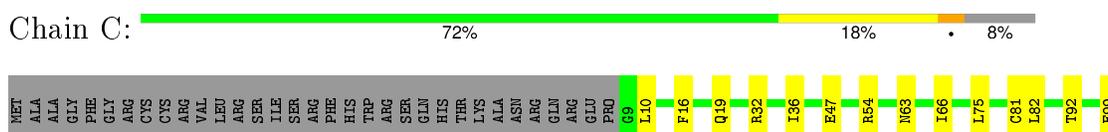
- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

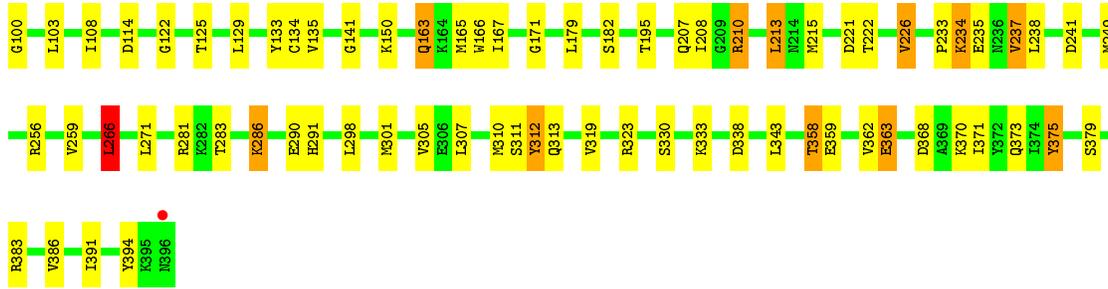


- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

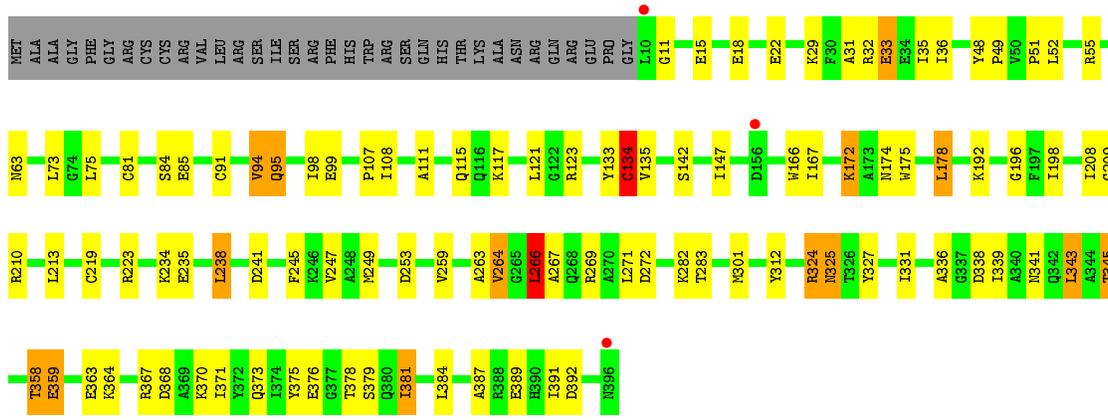


- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

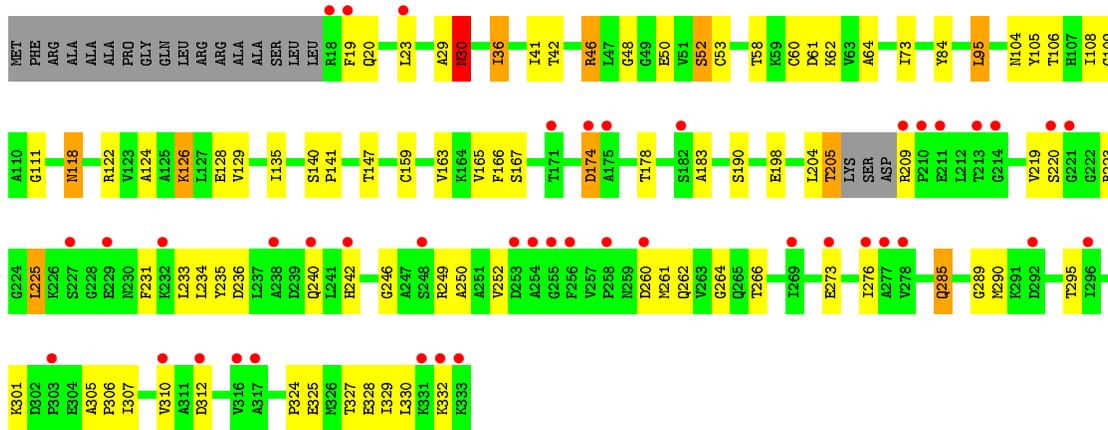




- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

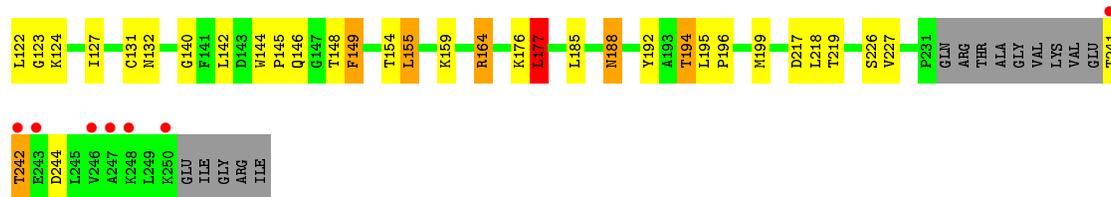


- Molecule 2: Electron transfer flavoprotein alpha-subunit, mitochondrial precursor



- 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)	Xtrriage
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 (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtrriage
Anisotropy	0.310	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Outliers	0 of 53814 reflections	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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: AMP, 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	0.74	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

The worst 5 of 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

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

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	S	23	0	12	1	0
5	A	53	0	31	7	0
5	B	53	0	31	3	0
5	C	53	0	31	5	0
5	D	53	0	31	4	0
5	R	53	0	31	4	0
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.

The worst 5 of 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	5: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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	384/421 (91%)	361 (94%)	22 (6%)	1 (0%)	46 79
1	B	385/421 (91%)	368 (96%)	15 (4%)	2 (0%)	34 69
1	C	386/421 (92%)	372 (96%)	12 (3%)	2 (0%)	34 69
1	D	385/421 (91%)	365 (95%)	20 (5%)	0	100 100
2	R	309/333 (93%)	270 (87%)	31 (10%)	8 (3%)	7 22
3	S	235/255 (92%)	205 (87%)	25 (11%)	5 (2%)	9 29
All	All	2084/2272 (92%)	1941 (93%)	125 (6%)	18 (1%)	21 55

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	C	234	LYS
3	S	218	LEU

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Mol	Chain	Res	Type
2	R	30	ASN
2	R	50	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/332 (86%)	259 (90%)	28 (10%)	10	28
1	B	288/332 (87%)	260 (90%)	28 (10%)	10	29
1	C	293/332 (88%)	257 (88%)	36 (12%)	6	18
1	D	296/332 (89%)	263 (89%)	33 (11%)	8	23
2	R	232/262 (88%)	204 (88%)	28 (12%)	6	18
3	S	183/213 (86%)	163 (89%)	20 (11%)	8	23
All	All	1579/1803 (88%)	1406 (89%)	173 (11%)	8	23

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	249	MET
1	D	94	VAL
3	S	111	LEU
1	C	259	VAL
1	C	358	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	313	GLN
1	D	19	GLN
3	S	70	GLN
1	C	349	GLN
1	C	373	GLN

### 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 carbohydrates 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
5	FAD	A	399	-	48,58,58	1.18	6 (12%)	54,89,89	2.35	12 (22%)
5	FAD	B	1399	-	48,58,58	1.28	6 (12%)	54,89,89	2.25	11 (20%)
5	FAD	C	2399	-	48,58,58	1.35	5 (10%)	54,89,89	2.17	9 (16%)
5	FAD	D	3399	-	48,58,58	1.26	5 (10%)	54,89,89	2.38	8 (14%)
5	FAD	R	599	-	48,58,58	1.25	6 (12%)	54,89,89	2.39	12 (22%)
4	AMP	S	600	-	20,25,25	1.01	1 (5%)	22,38,38	2.20	6 (27%)

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
5	FAD	A	399	-	-	0/30/50/50	0/6/6/6
5	FAD	B	1399	-	-	0/30/50/50	0/6/6/6
5	FAD	C	2399	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	D	3399	-	-	0/30/50/50	0/6/6/6
5	FAD	R	599	-	-	0/30/50/50	0/6/6/6
4	AMP	S	600	-	-	0/6/26/26	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	599	FAD	C5X-N5	2.05	1.38	1.35
5	A	399	FAD	C4-N3	2.06	1.36	1.33
5	B	1399	FAD	C2A-N1A	2.20	1.38	1.33
5	R	599	FAD	C10-N1	2.29	1.39	1.35
5	A	399	FAD	C5X-N5	2.34	1.39	1.35

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	599	FAD	N3A-C2A-N1A	-13.22	118.77	128.89
5	A	399	FAD	N3A-C2A-N1A	-12.48	119.34	128.89
5	B	1399	FAD	N3A-C2A-N1A	-11.75	119.90	128.89
5	D	3399	FAD	N3A-C2A-N1A	-11.54	120.06	128.89
5	C	2399	FAD	N3A-C2A-N1A	-10.55	120.81	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	399	FAD	7	0
5	B	1399	FAD	3	0
5	C	2399	FAD	5	0
5	D	3399	FAD	4	0
5	R	599	FAD	4	0
4	S	600	AMP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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 92	26, 37, 49, 57	0
1	B	387/421 (91%)	-0.44	3 (0%) 87 81	26, 40, 53, 62	0
1	C	388/421 (92%)	-0.55	1 (0%) 94 92	24, 37, 49, 60	0
1	D	387/421 (91%)	-0.52	3 (0%) 87 81	24, 37, 51, 60	0
2	R	313/333 (93%)	0.58	42 (13%) 4 2	43, 63, 91, 104	0
3	S	239/255 (93%)	0.05	10 (4%) 40 28	36, 53, 77, 111	0
All	All	2100/2272 (92%)	-0.28	60 (2%) 55 43	24, 41, 82, 111	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	333	LYS	6.3
2	R	220	SER	5.1
2	R	213	THR	4.9
2	R	303	PRO	4.8
2	R	242	HIS	4.6

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	FAD	C	2399	53/53	0.97	0.12	-0.34	29,33,36,37	0
5	FAD	B	1399	53/53	0.97	0.13	-0.35	29,35,41,42	0
5	FAD	R	599	53/53	0.91	0.17	-0.62	61,65,71,71	0
5	FAD	D	3399	53/53	0.97	0.11	-0.74	28,32,37,37	0
5	FAD	A	399	53/53	0.97	0.12	-0.90	27,33,35,36	0
4	AMP	S	600	23/23	0.96	0.12	-1.24	41,45,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.