



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:11 PM GMT

PDB ID : 1EGC
Title : STRUCTURE OF T255E, E376G MUTANT OF HUMAN MEDIUM CHAIN
ACYL-COA DEHYDROGENASE COMPLEXED WITH OCTANOYL-COA
Authors : Lee, H.J.; Wang, M.; Paschke, R.; Nandy, A.; Ghisla, S.; Kim, J.P.
Deposited on : 1996-04-11
Resolution : 2.60 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

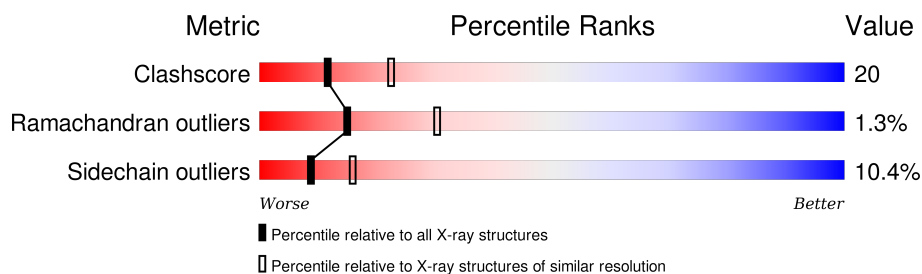
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	 55% 36% 7% .
1	B	396	 60% 33% 5% .
1	C	396	 63% 30% . .
1	D	396	 51% 39% 7% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12536 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.

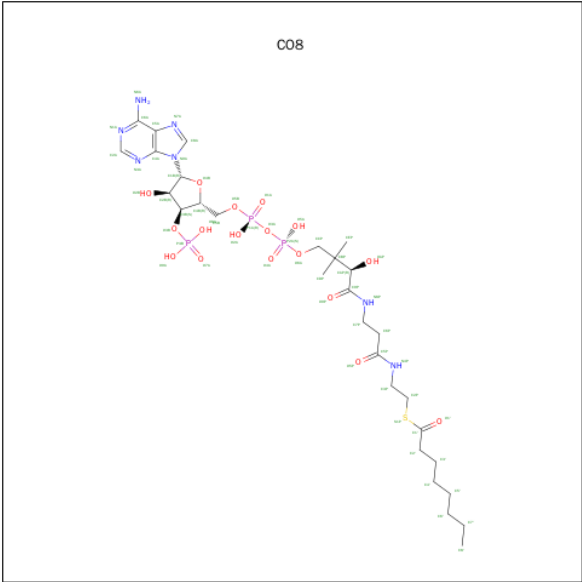
- Molecule 1 is a protein called MEDIUM CHAIN ACYL-COA DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2990	1892	515	565	18			
1	B	387	Total	C	N	O	S	0	0	0
			2990	1892	515	565	18			
1	C	387	Total	C	N	O	S	0	0	0
			2990	1892	515	565	18			
1	D	387	Total	C	N	O	S	5	0	0
			2990	1892	515	565	18			

There are 8 discrepancies between the modelled and reference sequences:

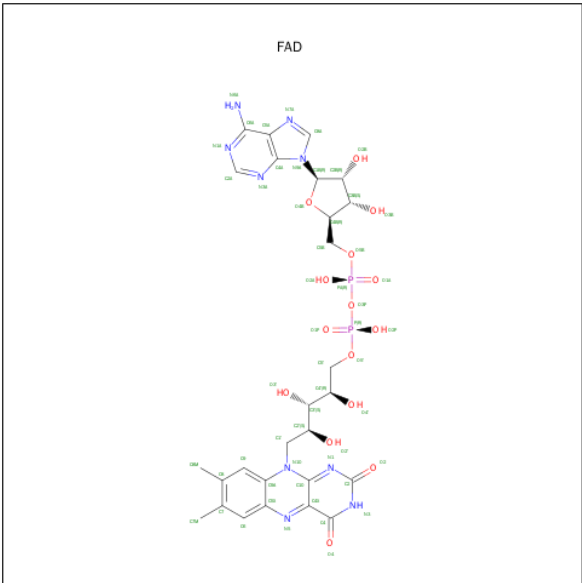
Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLU	THR	ENGINEERED	UNP P11310
A	376	GLY	GLU	ENGINEERED	UNP P11310
B	255	GLU	THR	ENGINEERED	UNP P11310
B	376	GLY	GLU	ENGINEERED	UNP P11310
C	255	GLU	THR	ENGINEERED	UNP P11310
C	376	GLY	GLU	ENGINEERED	UNP P11310
D	255	GLU	THR	ENGINEERED	UNP P11310
D	376	GLY	GLU	ENGINEERED	UNP P11310

- Molecule 2 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: C₂₉H₅₀N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

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



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

- Molecule 4 is water.

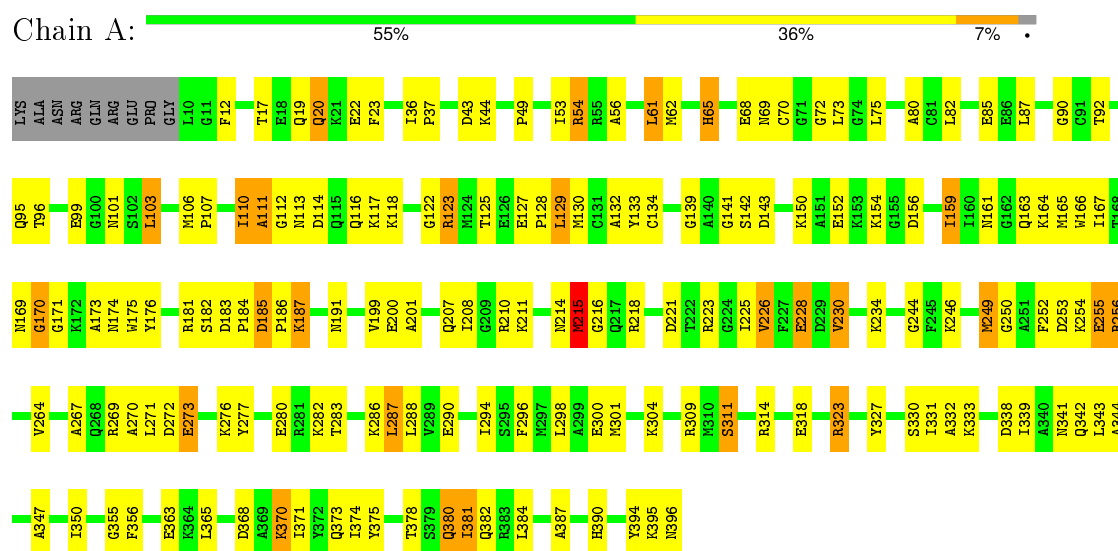
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	33	Total	O	0	0
			33	33		
4	C	41	Total	O	0	0
			41	41		
4	D	35	Total	O	0	0
			35	35		

3 Residue-property plots

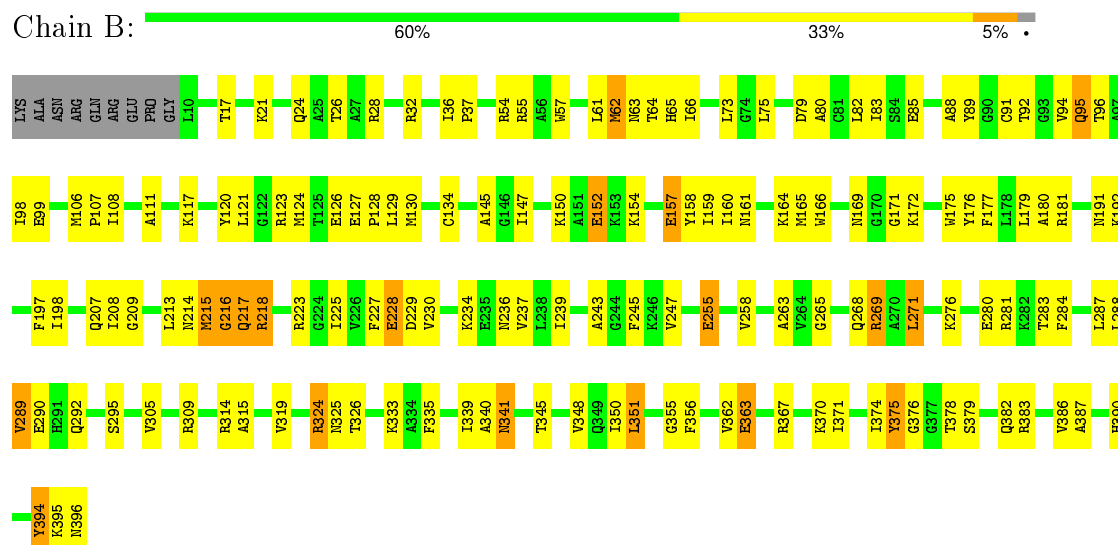
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

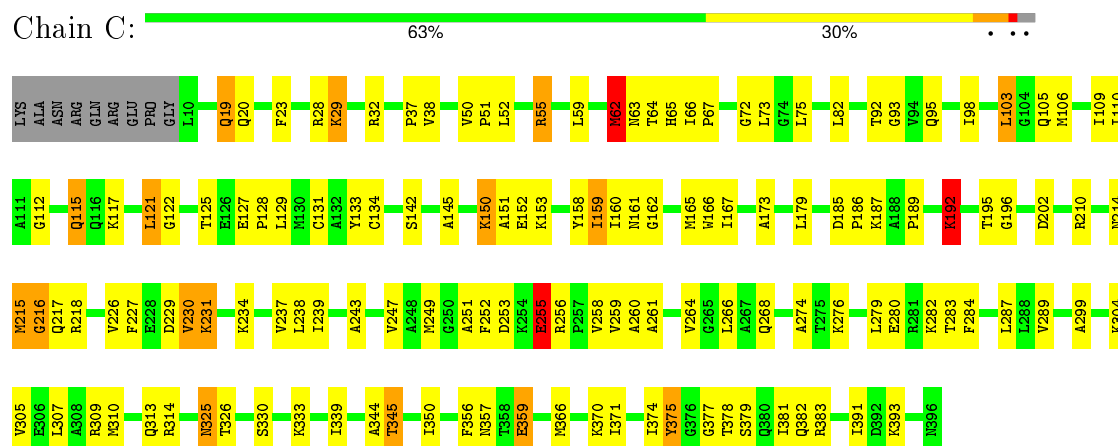
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE



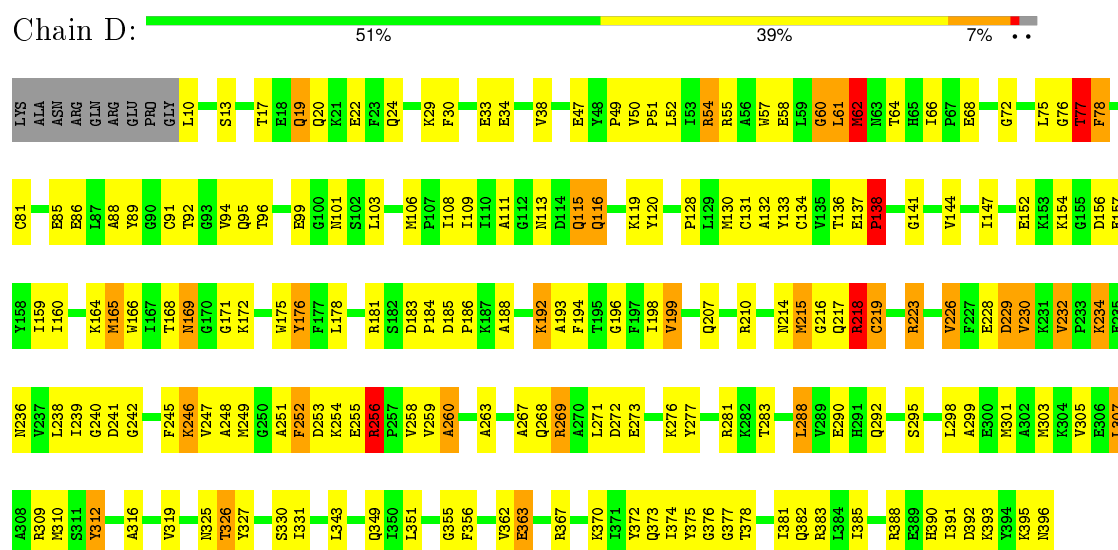
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE



• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE



• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.00 Å 170.00 Å 149.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12536	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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: CO8, 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	0.58	3/3045 (0.1%)	0.86	12/4102 (0.3%)
1	B	0.57	1/3045 (0.0%)	0.83	13/4102 (0.3%)
1	C	0.49	0/3045	0.77	7/4102 (0.2%)
1	D	0.56	2/3045 (0.1%)	0.82	10/4102 (0.2%)
All	All	0.55	6/12180 (0.0%)	0.82	42/16408 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	1
1	D	0	1
All	All	0	6

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	ASN	C-N	-8.13	1.15	1.34
1	D	260	ALA	C-N	7.39	1.51	1.34
1	A	230	VAL	C-N	7.13	1.50	1.34
1	A	170	GLY	C-N	7.04	1.45	1.33
1	A	226	VAL	C-N	-5.85	1.20	1.34

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ILE	CA-C-O	-12.21	94.45	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ILE	CB-CA-C	10.83	133.26	111.60
1	C	218	ARG	O-C-N	-10.66	105.64	122.70
1	A	111	ALA	CB-CA-C	10.20	125.39	110.10
1	D	77	THR	N-CA-CB	-9.95	91.40	110.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ILE	Mainchain,Peptide
1	A	170	GLY	Mainchain
1	A	230	VAL	Mainchain
1	C	230	VAL	Mainchain
1	D	64	THR	Mainchain

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	2990	0	2977	128	0
1	B	2990	0	2975	110	0
1	C	2990	0	2977	116	0
1	D	2990	0	2978	167	0
2	A	57	0	46	11	0
2	B	57	0	46	8	0
2	C	57	0	46	9	0
2	D	57	0	46	14	0
3	A	53	0	30	5	0
3	B	53	0	31	4	0
3	C	53	0	31	2	0
3	D	53	0	31	4	0
4	A	27	0	0	1	0
4	B	33	0	0	0	0
4	C	41	0	0	2	0
4	D	35	0	0	3	0
All	All	12536	0	12214	499	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 20.

The worst 5 of 499 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:C:274:ALA:HB1	1:C:350:ILE:HD11	1.29	1.13
1:C:216:GLY:HA3	1:D:356:PHE:HZ	1.12	1.11
1:C:216:GLY:HA3	1:D:356:PHE:CZ	1.89	1.07
1:D:256:ARG:HH11	1:D:256:ARG:CG	1.71	1.03
1:C:150:LYS:HD2	1:C:161:ASN:HB2	1.38	1.01

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	385/396 (97%)	344 (89%)	39 (10%)	2 (0%)	34	60
1	B	385/396 (97%)	351 (91%)	33 (9%)	1 (0%)	46	72
1	C	385/396 (97%)	351 (91%)	29 (8%)	5 (1%)	15	30
1	D	385/396 (97%)	334 (87%)	39 (10%)	12 (3%)	5	8
All	All	1540/1584 (97%)	1380 (90%)	140 (9%)	20 (1%)	15	30

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	61	LEU
1	D	77	THR
1	D	228	GLU
1	D	326	THR
1	A	141	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/310 (98%)	265 (88%)	38 (12%)	6	10
1	B	303/310 (98%)	274 (90%)	29 (10%)	10	20
1	C	303/310 (98%)	278 (92%)	25 (8%)	14	27
1	D	303/310 (98%)	269 (89%)	34 (11%)	7	13
All	All	1212/1240 (98%)	1086 (90%)	126 (10%)	9	16

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	SER
1	C	62	MET
1	D	256	ARG
1	B	324	ARG
1	B	375	TYR

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	B	380	GLN
1	C	105	GLN
1	D	349	GLN
1	C	19	GLN
1	C	63	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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$
3	FAD	A	399	-	48,58,58	1.67	9 (18%)	54,89,89	3.22	19 (35%)
2	CO8	A	400	-	49,59,59	1.56	6 (12%)	61,85,85	2.04	12 (19%)
3	FAD	B	399	-	48,58,58	1.34	5 (10%)	54,89,89	2.79	13 (24%)
2	CO8	B	400	-	49,59,59	1.29	5 (10%)	61,85,85	2.88	17 (27%)
3	FAD	C	399	-	48,58,58	1.85	9 (18%)	54,89,89	2.69	15 (27%)
2	CO8	C	400	-	49,59,59	1.26	4 (8%)	61,85,85	4.00	23 (37%)
3	FAD	D	399	-	48,58,58	1.59	8 (16%)	54,89,89	2.73	13 (24%)
2	CO8	D	400	-	49,59,59	1.31	3 (6%)	61,85,85	1.69	13 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	399	-	-	0/30/50/50	0/6/6/6
2	CO8	A	400	-	-	1/54/74/74	0/3/3/3
3	FAD	B	399	-	-	0/30/50/50	0/6/6/6
2	CO8	B	400	-	-	0/54/74/74	0/3/3/3
3	FAD	C	399	-	-	0/30/50/50	0/6/6/6
2	CO8	C	400	-	-	0/54/74/74	0/3/3/3
3	FAD	D	399	-	-	0/30/50/50	0/6/6/6
2	CO8	D	400	-	-	0/54/74/74	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	399	FAD	C1'-N10	-4.34	1.43	1.48
2	B	400	CO8	C1'-S1P	-3.66	1.68	1.76
3	A	399	FAD	O2B-C2B	-3.16	1.35	1.43
3	D	399	FAD	C1'-N10	-2.73	1.45	1.48
3	D	399	FAD	C8A-N7A	-2.71	1.29	1.34

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	CO8	O1'-C1'-C2'	-23.99	107.43	123.94
2	B	400	CO8	O1'-C1'-S1P	-12.78	112.69	122.83
2	B	400	CO8	C2B-C1B-N9A	-7.55	102.75	114.29
3	A	399	FAD	C4X-C10-N10	-7.47	116.12	120.52
2	A	400	CO8	O1'-C1'-S1P	-7.32	117.02	122.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	CO8	P2A-O6A-CCP-CBP

There are no ring outliers.

8 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	399	FAD	5	0
2	A	400	CO8	11	0
3	B	399	FAD	4	0
2	B	400	CO8	8	0
3	C	399	FAD	2	0
2	C	400	CO8	9	0
3	D	399	FAD	4	0
2	D	400	CO8	14	0

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.