Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:32 AM GMT

PDB ID	:	3MDE
Title	:	CRYSTAL STRUCTURES OF MEDIUM CHAIN ACYL-COA DEHYDROGENASE FROM PIG LIVER MITOCHONDRIA WITH AND WITHOUT SUBSTRATE
Authors	:	Kim, J.-J.P.; Wang, M.; Paschke, R.
Deposited on	:	1994-07-13
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

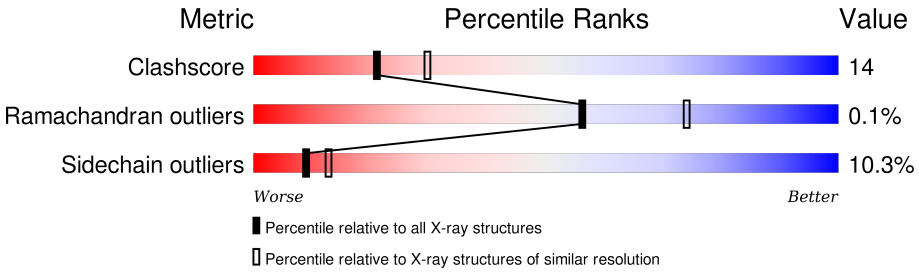
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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 <=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	385	67% 28% 5% •
1	B	385	67% 29% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6366 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.

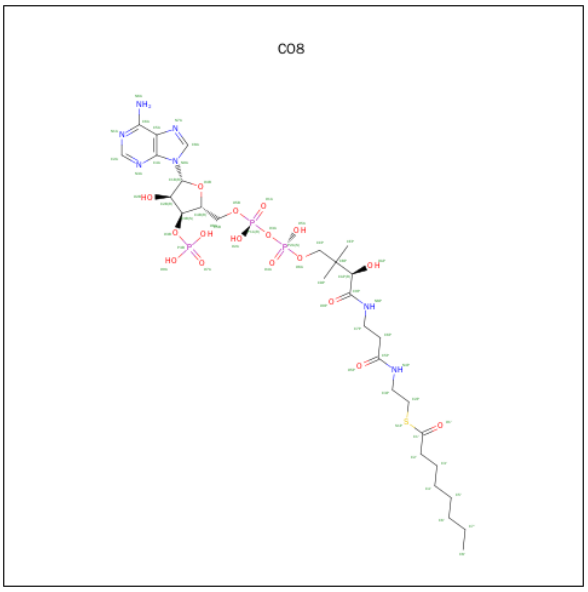
- Molecule 1 is a protein called MEDIUM CHAIN ACYL-COA DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2982	1891	514	563	14			
1	B	385	Total	C	N	O	S	0	0	0
			2982	1891	514	563	14			

There are 8 discrepancies between the modelled and reference sequences:

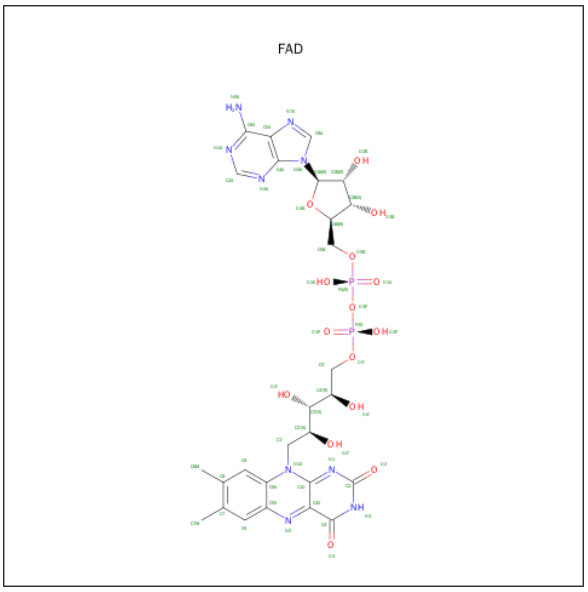
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLU	LYS	CONFLICT	UNP P41367
A	258	PRO	SER	CONFLICT	UNP P41367
A	280	GLU	GLY	CONFLICT	UNP P41367
A	306	GLU	ASP	CONFLICT	UNP P41367
B	15	GLU	LYS	CONFLICT	UNP P41367
B	258	PRO	SER	CONFLICT	UNP P41367
B	280	GLU	GLY	CONFLICT	UNP P41367
B	306	GLU	ASP	CONFLICT	UNP P41367

- Molecule 2 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$).



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		

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	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	100	Total	O	0	0
			100	100		
4	B	82	Total	O	0	0
			82	82		

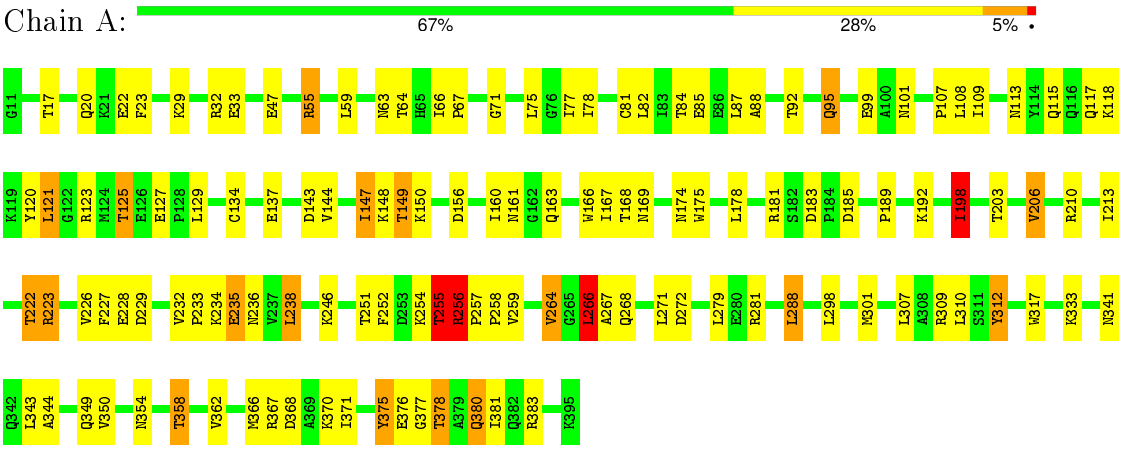
3 Residue-property plots (i)

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.

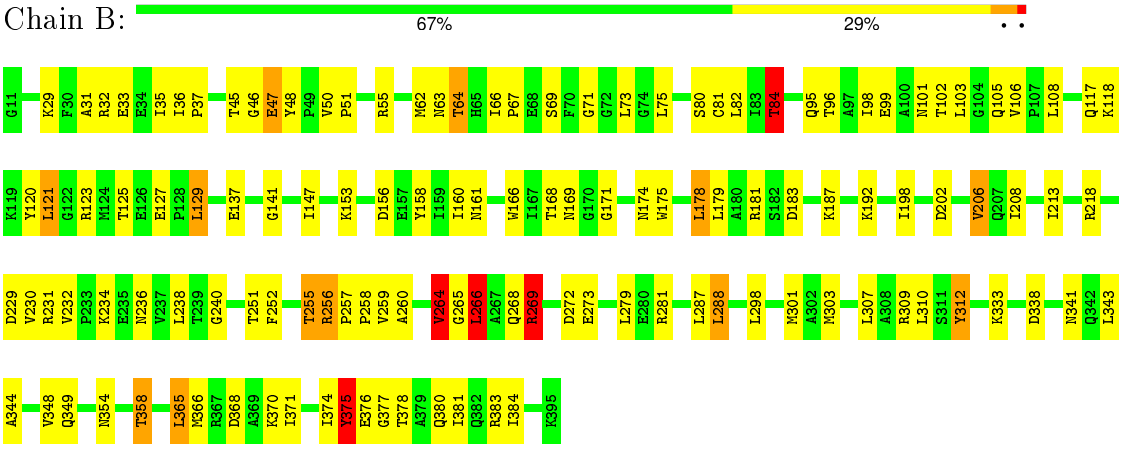
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain A:



• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	128.78Å 137.25Å 105.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6366	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.85	5/3039 (0.2%)	1.20	16/4101 (0.4%)
1	B	0.83	3/3039 (0.1%)	1.18	16/4101 (0.4%)
All	All	0.84	8/6078 (0.1%)	1.19	32/8202 (0.4%)

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	8
1	B	0	7
All	All	0	15

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	ILE	C-N	9.98	1.57	1.34
1	B	46	GLY	C-N	9.15	1.55	1.34
1	A	22	GLU	C-N	7.98	1.52	1.34
1	B	374	ILE	C-N	6.89	1.49	1.34
1	A	377	GLY	C-N	-6.28	1.19	1.34
1	A	362	VAL	C-N	5.90	1.47	1.34
1	A	107	PRO	C-N	-5.51	1.21	1.34
1	B	265	GLY	C-N	-5.08	1.22	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	256	ARG	NE-CZ-NH1	9.27	124.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	223	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	383	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	B	256	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	218	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	223	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	32	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	32	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	367	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	147	ILE	C-N-CA	-6.05	106.56	121.70
1	A	256	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	107	PRO	C-N-CA	5.92	136.49	121.70
1	B	231	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	272	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	B	266	LEU	O-C-N	-5.72	113.55	122.70
1	A	256	ARG	CD-NE-CZ	5.66	131.52	123.60
1	B	303	MET	CG-SD-CE	5.57	109.11	100.20
1	A	266	LEU	O-C-N	-5.54	113.84	122.70
1	B	338	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	272	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	240	GLY	O-C-N	5.41	131.35	122.70
1	B	269	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	32	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	264	VAL	O-C-N	-5.21	114.34	123.20
1	A	377	GLY	C-N-CA	5.20	134.70	121.70
1	B	202	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	143	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	383	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	210	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	147	ILE	O-C-N	5.02	130.73	122.70
1	B	272	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	THR	Mainchain
1	A	198	ILE	Mainchain
1	A	23	PHE	Mainchain
1	A	255	THR	Mainchain
1	A	264	VAL	Mainchain
1	A	266	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	350	VAL	Mainchain
1	A	47	GLU	Mainchain
1	B	178	LEU	Mainchain
1	B	264	VAL	Mainchain
1	B	266	LEU	Mainchain
1	B	269	ARG	Sidechain
1	B	375	TYR	Mainchain
1	B	47	GLU	Mainchain
1	B	84	THR	Mainchain

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	2982	0	2970	98	0
1	B	2982	0	2972	84	0
2	A	57	0	46	7	0
2	B	57	0	46	6	0
3	A	53	0	31	7	0
3	B	53	0	31	2	0
4	A	100	0	0	1	0
4	B	82	0	0	2	0
All	All	6366	0	6096	176	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 14.

All (176) 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:137:GLU:OE2	1:A:149:THR:HG23	1.66	0.95
1:A:123:ARG:HH11	1:A:174:ASN:HD21	1.15	0.92
1:A:266:LEU:C	1:A:266:LEU:HD12	1.91	0.91
1:B:108:LEU:HD23	1:B:121:LEU:HD13	1.55	0.88
1:B:108:LEU:HD11	1:B:198:ILE:HD11	1.60	0.84
1:A:63:ASN:HD21	1:A:101:ASN:HD22	1.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASN:HD21	1:B:101:ASN:HD22	1.26	0.82
1:B:266:LEU:HD12	1:B:266:LEU:C	2.00	0.82
1:B:268:GLN:HE21	1:B:309:ARG:HH22	1.32	0.78
1:B:378:THR:HG23	4:B:904:HOH:O	1.84	0.78
1:A:380:GLN:H	1:A:380:GLN:HE21	1.33	0.76
1:B:123:ARG:HH11	1:B:174:ASN:HD21	1.34	0.76
1:A:380:GLN:NE2	1:A:380:GLN:H	1.86	0.73
1:A:378:THR:HG22	1:A:381:ILE:H	1.53	0.73
1:A:213:ILE:O	1:B:358:THR:HB	1.91	0.71
1:B:174:ASN:HD22	1:B:175:TRP:HD1	1.39	0.71
1:A:378:THR:HG23	1:A:380:GLN:HE21	1.56	0.70
1:A:161:ASN:ND2	1:A:229:ASP:H	1.90	0.70
1:B:161:ASN:ND2	1:B:229:ASP:H	1.89	0.69
1:B:376:GLU:HG2	2:B:400:CO8:H2'2	1.76	0.68
1:B:268:GLN:NE2	1:B:309:ARG:HH22	1.91	0.68
1:A:370:LYS:HE2	1:B:348:VAL:HG22	1.76	0.67
1:A:266:LEU:C	1:A:266:LEU:CD1	2.64	0.66
1:A:378:THR:HG21	3:A:399:FAD:O2B	1.96	0.66
1:A:174:ASN:HD22	1:A:175:TRP:HD1	1.44	0.65
1:A:268:GLN:HE21	1:A:309:ARG:HH22	1.44	0.65
1:A:166:TRP:HZ2	1:B:354:ASN:HD22	1.45	0.64
1:A:376:GLU:H	2:A:400:CO8:H21	1.61	0.64
1:B:137:GLU:OE2	1:B:147:ILE:HG23	1.97	0.64
1:B:341:ASN:HD21	1:B:370:LYS:HA	1.61	0.64
1:A:266:LEU:HD12	1:A:266:LEU:O	1.97	0.63
1:B:71:GLY:HA3	1:B:125:THR:HG21	1.81	0.63
1:A:255:THR:O	1:A:258:PRO:HD2	1.98	0.63
2:B:400:CO8:H22	3:B:399:FAD:O2'	1.98	0.63
1:B:266:LEU:C	1:B:266:LEU:CD1	2.67	0.62
1:A:17:THR:H	1:A:20:GLN:HE21	1.48	0.61
1:A:281:ARG:HB3	1:A:288:LEU:HD22	1.80	0.61
1:B:160:ILE:HD11	1:B:232:VAL:HG11	1.83	0.60
1:B:158:TYR:HB2	1:B:232:VAL:HG13	1.83	0.60
1:B:96:THR:HG23	2:B:400:CO8:H6'1	1.82	0.60
1:B:256:ARG:HA	1:B:259:VAL:HG12	1.83	0.59
1:A:163:GLN:HG3	1:A:226:VAL:HG22	1.84	0.59
1:B:251:THR:O	1:B:255:THR:HB	2.02	0.59
1:A:109:ILE:HG13	1:A:121:LEU:HD21	1.84	0.59
1:A:381:ILE:HG21	2:A:400:CO8:H72	1.85	0.59
1:A:358:THR:HB	1:B:213:ILE:O	2.02	0.58
1:B:171:GLY:HA2	1:B:208:ILE:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLY:HA3	1:A:125:THR:HG21	1.86	0.58
1:A:341:ASN:HD21	1:A:370:LYS:HA	1.69	0.57
1:B:127:GLU:HB2	1:B:129:LEU:HD13	1.85	0.57
1:A:108:LEU:HD23	1:A:121:LEU:HD13	1.86	0.57
1:A:161:ASN:HD21	1:A:229:ASP:H	1.51	0.56
1:A:161:ASN:ND2	1:A:228:GLU:HA	2.20	0.56
1:A:115:GLN:HA	1:A:118:LYS:HE3	1.88	0.56
1:A:99:GLU:HB3	2:A:400:CO8:H7'1	1.88	0.56
1:A:123:ARG:NH1	1:A:174:ASN:HD21	1.97	0.56
1:A:380:GLN:N	1:A:380:GLN:NE2	2.53	0.56
1:B:117:GLN:O	1:B:121:LEU:HB2	2.06	0.56
1:A:63:ASN:HB3	1:A:66:ILE:HD12	1.88	0.56
1:B:99:GLU:HB3	2:B:400:CO8:H7'1	1.88	0.55
1:B:64:THR:HG23	1:B:75:LEU:HB2	1.88	0.55
1:A:380:GLN:HE22	1:B:349:GLN:HE21	1.55	0.55
1:B:108:LEU:HD11	1:B:198:ILE:CD1	2.35	0.55
1:A:123:ARG:HH11	1:A:174:ASN:ND2	1.96	0.55
1:B:281:ARG:HB3	1:B:288:LEU:HD22	1.88	0.54
1:A:251:THR:O	1:A:255:THR:HB	2.07	0.54
1:B:368:ASP:O	1:B:371:ILE:HG22	2.08	0.54
1:A:113:ASN:O	1:A:117:GLN:HG3	2.07	0.54
1:A:161:ASN:HA	1:A:227:PHE:O	2.07	0.53
1:A:378:THR:HG23	1:A:380:GLN:NE2	2.21	0.53
1:A:349:GLN:HE21	1:B:380:GLN:HE22	1.57	0.52
1:B:268:GLN:HE21	1:B:309:ARG:NH2	2.03	0.52
1:A:17:THR:H	1:A:20:GLN:NE2	2.06	0.52
1:A:77:ILE:HD11	1:A:254:LYS:HD3	1.91	0.52
1:B:36:ILE:N	1:B:37:PRO:HD2	2.24	0.52
1:B:80:SER:O	1:B:84:THR:HB	2.10	0.52
1:B:45:THR:OG1	1:B:47:GLU:HG3	2.10	0.52
1:A:252:PHE:O	1:A:256:ARG:HB2	2.11	0.51
1:A:203:THR:O	1:A:206:VAL:HG13	2.10	0.51
1:A:78:ILE:HD11	1:A:317:TRP:HA	1.93	0.51
1:A:256:ARG:HG3	1:A:333:LYS:HG3	1.92	0.50
1:A:378:THR:CG2	1:A:380:GLN:HE21	2.23	0.50
1:A:108:LEU:HD21	1:A:120:TYR:HB2	1.93	0.50
1:A:301:MET:HG2	1:A:343:LEU:HG	1.93	0.50
1:B:50:VAL:HB	1:B:51:PRO:HD3	1.94	0.50
1:A:117:GLN:O	1:A:121:LEU:HB2	2.12	0.49
1:A:160:ILE:HD12	1:A:232:VAL:HG11	1.94	0.49
1:A:168:THR:O	1:A:169:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ALA:O	1:B:264:VAL:HG13	2.13	0.49
1:A:84:THR:HG21	1:A:258:PRO:O	2.13	0.49
1:A:160:ILE:CD1	1:A:232:VAL:HG11	2.43	0.49
1:B:102:THR:O	1:B:106:VAL:HG23	2.13	0.49
1:B:252:PHE:O	1:B:256:ARG:HB2	2.12	0.48
1:B:269:ARG:HD2	1:B:273:GLU:OE2	2.14	0.48
1:B:255:THR:O	1:B:258:PRO:HD2	2.14	0.48
1:A:189:PRO:HG2	1:A:192:LYS:HE3	1.96	0.47
1:B:255:THR:HG23	1:B:376:GLU:OE2	2.13	0.47
1:A:63:ASN:HD21	1:A:101:ASN:ND2	2.03	0.47
1:B:187:LYS:N	1:B:187:LYS:HD2	2.30	0.47
1:A:63:ASN:HB3	1:A:66:ILE:CD1	2.45	0.47
1:A:252:PHE:CZ	2:A:400:CO8:H31	2.49	0.47
1:A:256:ARG:N	1:A:257:PRO:CD	2.78	0.47
2:A:400:CO8:H22	3:A:399:FAD:O2'	2.14	0.47
1:A:257:PRO:HB2	1:A:258:PRO:HD3	1.96	0.46
1:A:354:ASN:ND2	1:B:166:TRP:HZ2	2.14	0.46
1:A:341:ASN:ND2	4:A:840:HOH:O	2.48	0.46
1:B:31:ALA:HA	1:B:35:ILE:HD12	1.98	0.46
3:A:399:FAD:H51A	1:B:288:LEU:HD21	1.97	0.46
1:A:376:GLU:HG2	2:A:400:CO8:H2'2	1.98	0.46
1:B:103:LEU:HD21	2:B:400:CO8:H2'1	1.96	0.46
1:A:375:TYR:HB2	2:A:400:CO8:O1'	2.15	0.46
1:B:206:VAL:HG12	1:B:230:VAL:HG21	1.97	0.46
1:B:96:THR:HG22	1:B:168:THR:HG21	1.98	0.45
1:B:269:ARG:HG3	1:B:365:LEU:HD21	1.97	0.45
1:A:137:GLU:OE2	1:A:147:ILE:HB	2.17	0.45
1:B:62:MET:HG3	1:B:98:ILE:HG23	1.99	0.45
1:A:375:TYR:O	1:A:376:GLU:HB2	2.17	0.44
1:A:120:TYR:CE1	1:A:198:ILE:HD11	2.51	0.44
1:A:344:ALA:HB1	1:A:366:MET:HA	1.99	0.44
1:B:344:ALA:HB1	1:B:366:MET:HA	2.00	0.44
1:A:55:ARG:O	1:A:59:LEU:HB2	2.18	0.44
1:B:178:LEU:HD13	1:B:178:LEU:C	2.37	0.44
1:A:368:ASP:O	1:A:371:ILE:HG22	2.18	0.44
1:B:256:ARG:N	1:B:257:PRO:CD	2.81	0.44
1:A:161:ASN:HD22	1:A:228:GLU:HA	1.81	0.43
1:B:108:LEU:HD23	1:B:121:LEU:CD1	2.37	0.43
1:B:81:CYS:HB3	1:B:312:TYR:CE1	2.52	0.43
1:A:255:THR:HG23	1:A:376:GLU:OE2	2.18	0.43
1:A:95:GLN:HB3	1:A:95:GLN:HE21	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD22	2:B:400:CO8:H5'2	2.00	0.43
1:B:63:ASN:ND2	1:B:105:GLN:OE1	2.52	0.43
1:A:88:ALA:HB1	1:A:92:THR:HG22	2.01	0.43
1:B:181:ARG:NH1	1:B:183:ASP:O	2.46	0.43
1:B:108:LEU:CD1	1:B:198:ILE:HD11	2.41	0.43
1:A:81:CYS:HB3	1:A:312:TYR:CE1	2.53	0.43
1:B:301:MET:HG2	1:B:343:LEU:HG	2.01	0.43
1:B:178:LEU:HD13	1:B:179:LEU:N	2.35	0.42
1:B:123:ARG:HH11	1:B:174:ASN:ND2	2.10	0.42
1:A:371:ILE:HD13	3:A:399:FAD:HM83	2.01	0.42
1:A:85:GLU:HG3	1:A:264:VAL:HG22	2.02	0.42
1:A:66:ILE:HA	1:A:67:PRO:HD3	1.83	0.42
1:B:108:LEU:HD21	1:B:120:TYR:HB2	2.02	0.42
1:A:29:LYS:HZ2	1:A:33:GLU:CD	2.23	0.42
1:B:381:ILE:HD13	1:B:384:ILE:HD12	2.02	0.42
1:A:222:THR:C	1:A:223:ARG:HG3	2.39	0.42
1:B:371:ILE:CD1	3:B:399:FAD:HM83	2.49	0.42
1:B:255:THR:C	1:B:258:PRO:HD2	2.40	0.42
1:B:29:LYS:O	1:B:33:GLU:HB2	2.20	0.42
1:B:269:ARG:O	1:B:273:GLU:HG2	2.21	0.41
1:A:354:ASN:HD22	1:B:166:TRP:HZ2	1.67	0.41
1:A:380:GLN:N	1:A:380:GLN:HE21	2.11	0.41
1:B:63:ASN:HB3	1:B:66:ILE:HD12	2.03	0.41
1:A:267:ALA:HB1	1:A:343:LEU:HD22	2.02	0.41
1:B:181:ARG:NH2	4:B:965:HOH:O	2.53	0.41
1:B:375:TYR:CD1	1:B:375:TYR:C	2.93	0.41
1:B:257:PRO:HB2	1:B:258:PRO:HD3	2.03	0.41
1:A:233:PRO:HB2	1:A:235:GLU:HG2	2.02	0.41
1:A:181:ARG:NH2	1:A:185:ASP:O	2.53	0.41
1:B:64:THR:HG23	1:B:75:LEU:CB	2.49	0.41
1:B:66:ILE:HA	1:B:67:PRO:HD3	1.90	0.41
1:A:378:THR:CG2	3:A:399:FAD:O2B	2.66	0.41
1:A:371:ILE:CD1	3:A:399:FAD:HM83	2.51	0.41
3:A:399:FAD:O3B	1:B:349:GLN:O	2.36	0.41
1:A:167:ILE:O	1:A:222:THR:HA	2.20	0.41
1:A:181:ARG:NE	1:A:183:ASP:O	2.54	0.41
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.63	0.41
1:A:120:TYR:CE2	1:A:198:ILE:HG12	2.56	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD23	1.88	0.41
1:A:271:LEU:HD13	1:A:301:MET:HB3	2.02	0.40
1:B:48:TYR:OH	1:B:169:ASN:ND2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:HA	1:A:150:LYS:HD2	1.91	0.40
1:B:310:LEU:HA	1:B:310:LEU:HD12	1.94	0.40
1:A:134:CYS:HA	1:A:167:ILE:HD12	2.03	0.40
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.96	0.40
1:B:333:LYS:NZ	1:B:377:GLY:O	2.50	0.40
1:A:178:LEU:C	1:A:178:LEU:HD13	2.42	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	383/385 (100%)	377 (98%)	6 (2%)	0	100 100
1	B	383/385 (100%)	376 (98%)	6 (2%)	1 (0%)	46 63
All	All	766/770 (100%)	753 (98%)	12 (2%)	1 (0%)	56 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	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	301/301 (100%)	266 (88%)	35 (12%)	7 9
1	B	301/301 (100%)	274 (91%)	27 (9%)	12 17
All	All	602/602 (100%)	540 (90%)	62 (10%)	9 13

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	64	THR
1	A	75	LEU
1	A	82	LEU
1	A	87	LEU
1	A	95	GLN
1	A	121	LEU
1	A	125	THR
1	A	127	GLU
1	A	129	LEU
1	A	144	VAL
1	A	148	LYS
1	A	156	ASP
1	A	198	ILE
1	A	206	VAL
1	A	222	THR
1	A	234	LYS
1	A	235	GLU
1	A	236	ASN
1	A	238	LEU
1	A	246	LYS
1	A	255	THR
1	A	256	ARG
1	A	259	VAL
1	A	266	LEU
1	A	279	LEU
1	A	288	LEU
1	A	298	LEU
1	A	307	LEU
1	A	310	LEU
1	A	312	TYR
1	A	358	THR
1	A	375	TYR
1	A	378	THR
1	A	380	GLN

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Mol	Chain	Res	Type
1	B	55	ARG
1	B	64	THR
1	B	69	SER
1	B	73	LEU
1	B	82	LEU
1	B	84	THR
1	B	95	GLN
1	B	118	LYS
1	B	121	LEU
1	B	129	LEU
1	B	153	LYS
1	B	156	ASP
1	B	192	LYS
1	B	206	VAL
1	B	234	LYS
1	B	236	ASN
1	B	255	THR
1	B	266	LEU
1	B	279	LEU
1	B	287	LEU
1	B	288	LEU
1	B	298	LEU
1	B	307	LEU
1	B	312	TYR
1	B	358	THR
1	B	365	LEU
1	B	375	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	63	ASN
1	A	95	GLN
1	A	105	GLN
1	A	161	ASN
1	A	169	ASN
1	A	174	ASN
1	A	236	ASN
1	A	268	GLN
1	A	313	GLN
1	A	341	ASN

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Mol	Chain	Res	Type
1	A	354	ASN
1	A	373	GLN
1	A	380	GLN
1	B	20	GLN
1	B	63	ASN
1	B	105	GLN
1	B	161	ASN
1	B	163	GLN
1	B	169	ASN
1	B	174	ASN
1	B	207	GLN
1	B	236	ASN
1	B	268	GLN
1	B	313	GLN
1	B	341	ASN
1	B	354	ASN
1	B	373	GLN
1	B	380	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

4 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	1.16	3 (6%)	54,89,89	1.93	7 (12%)
2	CO8	A	400	-	49,59,59	0.89	2 (4%)	61,85,85	3.26	15 (24%)
3	FAD	B	399	-	48,58,58	1.24	3 (6%)	54,89,89	1.79	6 (11%)
2	CO8	B	400	-	49,59,59	0.93	2 (4%)	61,85,85	3.04	15 (24%)

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	-	-	0/54/74/74	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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	CO8	C9P-N8P	2.16	1.38	1.33
3	B	399	FAD	C4-C4X	2.44	1.46	1.41
3	A	399	FAD	C4-C4X	2.45	1.46	1.41
2	B	400	CO8	C5P-N4P	2.49	1.39	1.33
3	A	399	FAD	C4-N3	2.92	1.38	1.33
2	A	400	CO8	C5P-N4P	2.93	1.40	1.33
2	B	400	CO8	C9P-N8P	2.94	1.39	1.33
3	B	399	FAD	C4-N3	3.23	1.39	1.33
3	A	399	FAD	C4X-N5	4.59	1.40	1.33
3	B	399	FAD	C4X-N5	5.35	1.41	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	CO8	O1'-C1'-S1P	-14.20	111.57	122.83
2	B	400	CO8	O1'-C1'-S1P	-12.15	113.19	122.83
2	A	400	CO8	C3P-N4P-C5P	-5.94	111.10	122.79
3	A	399	FAD	C1'-N10-C9A	-5.39	112.81	118.86
3	A	399	FAD	P-O3P-PA	-5.12	118.36	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	CO8	C3P-N4P-C5P	-5.10	112.76	122.79
3	A	399	FAD	C4X-C4-N3	-5.04	116.70	123.59
3	B	399	FAD	C1'-N10-C9A	-4.85	113.41	118.86
2	B	400	CO8	C7P-N8P-C9P	-4.81	113.00	122.53
2	B	400	CO8	P2A-O3A-P1A	-4.76	119.36	132.73
3	B	399	FAD	C4X-C4-N3	-4.74	117.11	123.59
3	B	399	FAD	P-O3P-PA	-4.32	120.59	132.73
2	A	400	CO8	P2A-O3A-P1A	-4.26	120.77	132.73
3	A	399	FAD	C4X-C10-N10	-3.80	118.28	120.52
2	A	400	CO8	C2B-C1B-N9A	-3.61	108.77	114.29
2	B	400	CO8	O5P-C5P-C6P	-3.58	115.80	121.98
2	B	400	CO8	O9P-C9P-N8P	-3.58	115.90	123.08
3	B	399	FAD	C4X-C10-N10	-3.54	118.43	120.52
3	A	399	FAD	O4'-C4'-C5'	-3.00	103.65	110.19
2	A	400	CO8	C1B-N9A-C4A	-2.97	122.46	126.94
2	A	400	CO8	C7P-N8P-C9P	-2.97	116.66	122.53
2	B	400	CO8	C1B-N9A-C4A	-2.93	122.52	126.94
2	A	400	CO8	O5P-C5P-C6P	-2.91	116.95	121.98
2	B	400	CO8	CDP-CBP-CCP	-2.82	104.84	108.50
2	B	400	CO8	C2B-C1B-N9A	-2.54	110.41	114.29
3	A	399	FAD	C5X-C9A-N10	-2.25	115.91	117.62
2	A	400	CO8	O9P-C9P-N8P	-2.12	118.83	123.08
2	B	400	CO8	O5P-C5P-N4P	2.04	126.99	122.94
2	A	400	CO8	O5P-C5P-N4P	2.10	127.10	122.94
3	B	399	FAD	C4X-N5-C5X	2.11	119.19	116.76
2	A	400	CO8	O4B-C1B-N9A	2.70	113.75	108.10
2	A	400	CO8	CAP-C9P-N8P	3.19	123.54	116.47
2	B	400	CO8	CAP-C9P-N8P	4.12	125.59	116.47
2	B	400	CO8	O6A-CCP-CBP	5.70	119.71	110.55
2	A	400	CO8	O3A-P2A-O6A	5.79	118.31	102.94
2	B	400	CO8	O3A-P2A-O6A	5.95	118.72	102.94
2	A	400	CO8	O6A-CCP-CBP	6.79	121.46	110.55
2	B	400	CO8	P3B-O3B-C3B	7.54	139.63	121.56
3	B	399	FAD	C4-N3-C2	7.72	121.92	115.25
3	A	399	FAD	C4-N3-C2	8.00	122.16	115.25
2	A	400	CO8	P3B-O3B-C3B	8.92	142.96	121.56
2	B	400	CO8	C2'-C1'-S1P	10.97	123.22	113.36
2	A	400	CO8	C2'-C1'-S1P	11.98	124.14	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	399	FAD	7	0
2	A	400	CO8	7	0
3	B	399	FAD	2	0
2	B	400	CO8	6	0

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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