



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:33 PM UTC

PDB ID : 3MDE / pdb_00003mde
Title : CRYSTAL STRUCTURES OF MEDIUM CHAIN ACYL-COA DEHYDROGENASE FROM PIG LIVER MITOCHONDRIA WITH AND WITHOUT SUBSTRATE
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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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

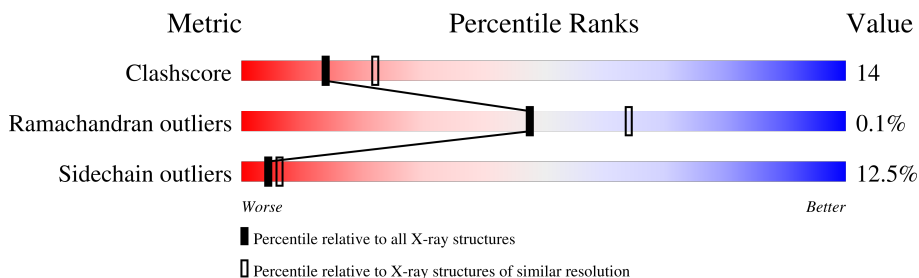
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	385	 66% 27% 5% •
1	B	385	 66% 27% 6% •

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.

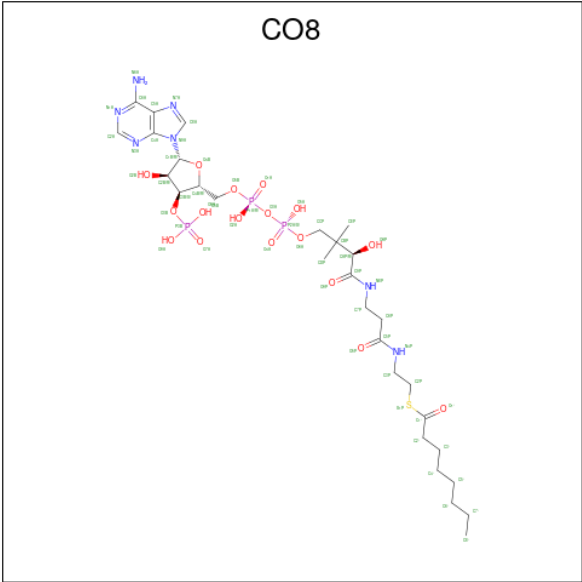
- Molecule 1 is a protein called MEDIUM CHAIN ACYL-COA DEHYDROGENASE.

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:

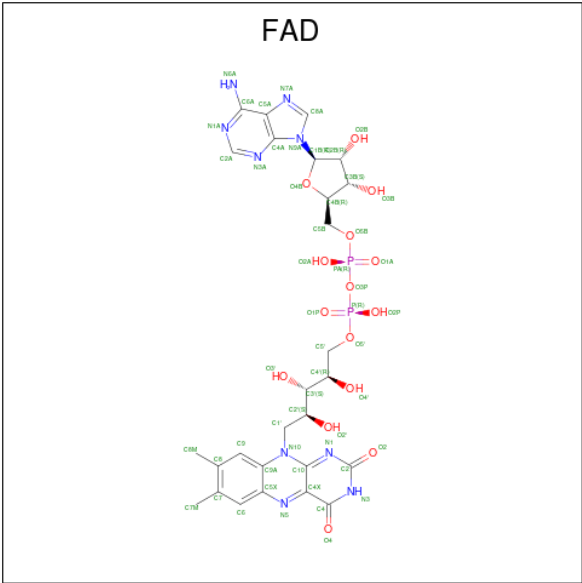
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLU	LYS	conflict	UNP P41367
A	258	PRO	SER	conflict	UNP P41367
A	280	GLU	GLY	conflict	UNP P41367
A	306	GLU	ASP	conflict	UNP P41367
B	15	GLU	LYS	conflict	UNP P41367
B	258	PRO	SER	conflict	UNP P41367
B	280	GLU	GLY	conflict	UNP P41367
B	306	GLU	ASP	conflict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

- Molecule 2 is OCTANOYL-COENZYME A (CCD ID: 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 (CCD ID: 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		

- Molecule 4 is water.

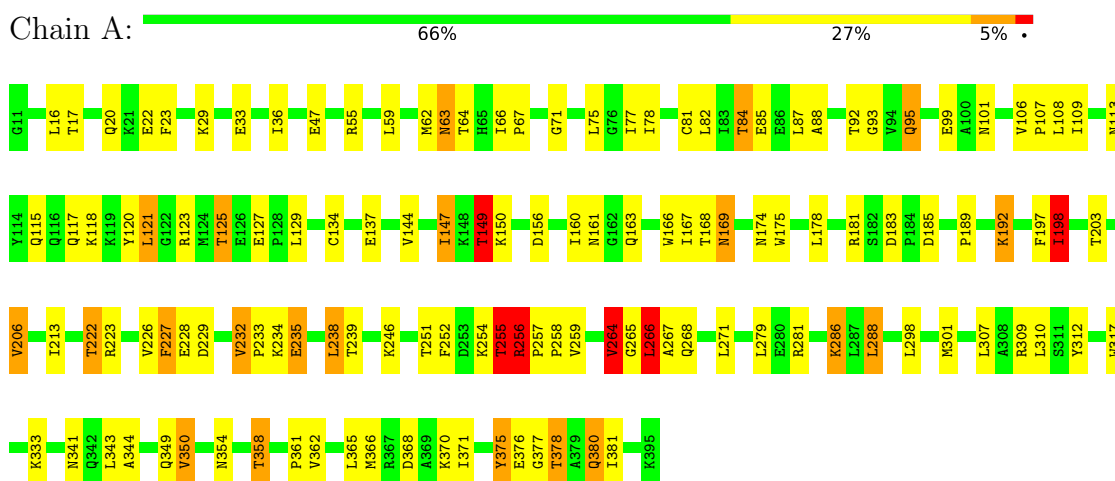
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total 100	O 100	0	0
4	B	82	Total 82	O 82	0	0

3 Residue-property plots

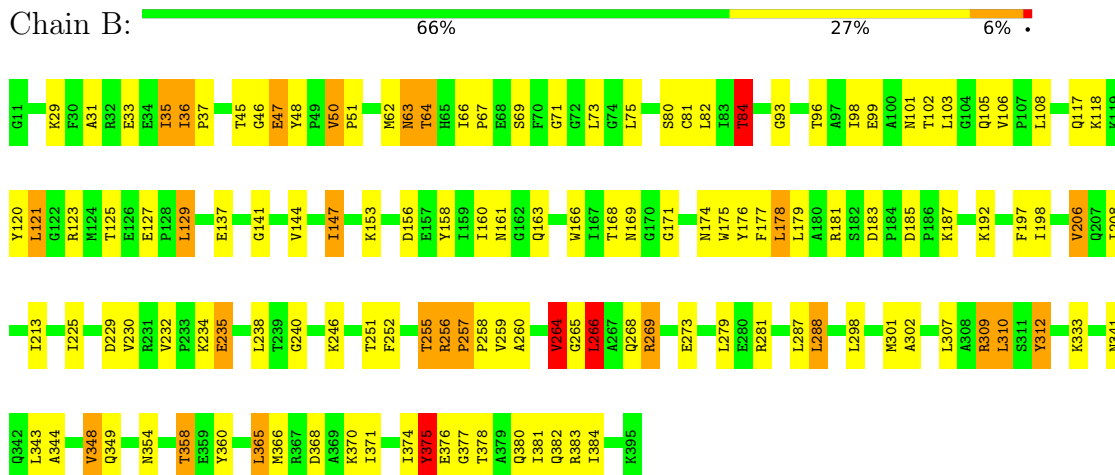
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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: FAD, CO8

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	1.09	11/3039 (0.4%)	1.61	32/4101 (0.8%)
1	B	1.06	11/3039 (0.4%)	1.54	27/4101 (0.7%)
All	All	1.07	22/6078 (0.4%)	1.58	59/8202 (0.7%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	GLY	C-N	16.63	1.55	1.33
1	A	147	ILE	C-N	14.40	1.57	1.33
1	A	22	GLU	C-N	14.20	1.52	1.33
1	B	374	ILE	C-N	11.54	1.49	1.33
1	A	377	GLY	C-N	-10.38	1.19	1.33
1	A	362	VAL	C-N	9.91	1.47	1.33
1	A	107	PRO	C-N	-9.23	1.21	1.33
1	A	36	ILE	CA-CB	8.90	1.58	1.54
1	B	302	ALA	C-N	-8.51	1.23	1.33
1	B	265	GLY	C-N	-7.89	1.22	1.33
1	A	227	PHE	C-N	7.66	1.43	1.33
1	A	286	LYS	C-N	-7.34	1.23	1.33
1	B	36	ILE	CA-CB	7.10	1.57	1.54
1	A	265	GLY	C-N	-6.80	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	VAL	C-N	6.46	1.41	1.33
1	B	177	PHE	C-N	-6.30	1.25	1.33
1	B	309	ARG	C-N	-6.30	1.25	1.33
1	B	240	GLY	C-N	-6.06	1.24	1.33
1	B	235	GLU	C-N	5.98	1.41	1.33
1	A	63	ASN	C-N	-5.66	1.26	1.34
1	B	382	GLN	C-N	5.66	1.41	1.33
1	A	266	LEU	C-N	5.06	1.41	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	PRO	CA-C-N	11.41	136.49	120.29
1	A	107	PRO	C-N-CA	11.41	136.49	120.29
1	A	147	ILE	CA-C-N	-9.98	106.56	122.23
1	A	147	ILE	C-N-CA	-9.98	106.56	122.23
1	A	377	GLY	CA-C-N	9.79	134.70	120.90
1	A	377	GLY	C-N-CA	9.79	134.70	120.90
1	A	227	PHE	CA-C-N	-9.05	110.24	123.00
1	A	227	PHE	C-N-CA	-9.05	110.24	123.00
1	A	63	ASN	CA-C-N	8.06	131.89	120.28
1	A	63	ASN	C-N-CA	8.06	131.89	120.28
1	A	197	PHE	CA-C-N	-7.99	112.73	123.12
1	A	197	PHE	C-N-CA	-7.99	112.73	123.12
1	A	147	ILE	O-C-N	7.87	130.73	122.62
1	B	265	GLY	CA-C-N	7.64	133.67	120.68
1	B	265	GLY	C-N-CA	7.64	133.67	120.68
1	B	240	GLY	O-C-N	7.38	131.35	123.23
1	B	197	PHE	CA-CB-CG	7.13	120.93	113.80
1	B	309	ARG	CA-C-N	7.10	130.37	120.29
1	B	309	ARG	C-N-CA	7.10	130.37	120.29
1	A	286	LYS	CA-C-N	6.68	130.24	120.82
1	A	286	LYS	C-N-CA	6.68	130.24	120.82
1	B	302	ALA	CA-C-N	6.67	129.11	120.44
1	B	302	ALA	C-N-CA	6.67	129.11	120.44
1	B	266	LEU	O-C-N	-6.55	113.55	122.33
1	B	374	ILE	N-CA-C	6.52	116.77	111.62
1	A	22	GLU	CA-C-N	-6.43	111.58	120.38
1	A	22	GLU	C-N-CA	-6.43	111.58	120.38
1	A	266	LEU	O-C-N	-6.25	113.84	122.46
1	B	374	ILE	O-C-N	6.21	126.76	121.98
1	A	264	VAL	O-C-N	-6.17	114.97	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	THR	O-C-N	-6.16	115.03	122.48
1	A	169	ASN	CA-CB-CG	6.03	118.63	112.60
1	B	374	ILE	CA-C-N	-6.02	109.97	122.07
1	B	374	ILE	C-N-CA	-6.02	109.97	122.07
1	B	360	TYR	CB-CA-C	5.97	118.10	109.09
1	B	264	VAL	O-C-N	-5.96	114.34	122.26
1	A	197	PHE	CA-CB-CG	5.90	119.70	113.80
1	A	255	THR	CA-C-N	5.84	127.02	119.78
1	A	255	THR	C-N-CA	5.84	127.02	119.78
1	A	106	VAL	O-C-N	5.83	124.15	120.42
1	B	63	ASN	CA-C-N	5.38	128.23	120.38
1	B	63	ASN	C-N-CA	5.38	128.23	120.38
1	B	93	GLY	N-CA-C	-5.36	106.00	112.49
1	B	383	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	A	362	VAL	CA-C-N	-5.32	111.84	120.72
1	A	362	VAL	C-N-CA	-5.32	111.84	120.72
1	B	176	TYR	CA-C-N	-5.30	114.71	122.19
1	B	176	TYR	C-N-CA	-5.30	114.71	122.19
1	A	361	PRO	N-CA-C	5.21	121.30	114.27
1	A	93	GLY	O-C-N	5.19	127.18	122.19
1	B	185	ASP	O-C-N	5.16	125.80	121.31
1	B	50	VAL	O-C-N	5.13	123.70	120.42
1	A	265	GLY	CA-C-N	5.13	130.11	121.14
1	A	265	GLY	C-N-CA	5.13	130.11	121.14
1	B	46	GLY	CA-C-N	-5.11	111.45	121.06
1	B	46	GLY	C-N-CA	-5.11	111.45	121.06
1	B	257	PRO	CB-CA-C	5.10	117.14	110.92
1	A	256	ARG	CD-NE-CZ	5.09	131.52	124.40
1	B	35	ILE	N-CA-C	5.05	115.17	110.42

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
1	A	350	VAL	Mainchain
1	A	47	GLU	Mainchain

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Mol	Chain	Res	Type	Group
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	2972	99	0
1	B	2982	0	2974	83	0
2	A	57	0	46	7	0
2	B	57	0	46	7	0
3	A	53	0	31	5	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	6100	177	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 (177) 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:266:LEU:C	1:A:266:LEU:HD12	1.91	0.95
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:B:108:LEU:HD23	1:B:121:LEU:HD13	1.55	0.88
1:B:266:LEU:C	1:B:266:LEU:HD12	2.00	0.86
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
1:B:63:ASN:HD21	1:B:101:ASN:HD22	1.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:380:GLN:NE2	1.86	0.73
1:A:378:THR:HG22	1:A:381:ILE:H	1.53	0.73
1:A:266:LEU:C	1:A:266:LEU:CD1	2.64	0.71
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:B:266:LEU:C	1:B:266:LEU:CD1	2.67	0.67
1:A:370:LYS:HE2	1:B:348:VAL:HG22	1.76	0.67
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: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:158:TYR:HB2	1:B:232:VAL:HG13	1.83	0.60
1:B:160:ILE:HD11	1:B:232:VAL:HG11	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:A:109:ILE:HG13	1:A:121:LEU:HD21	1.84	0.59
1:B:251:THR:O	1:B:255:THR:HB	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE2	1:A:380:GLN:N	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:64:THR:HG23	1:B:75:LEU:HB2	1.88	0.55
1:B:99:GLU:HB3	2:B:400:CO8:H7'1	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
2:B:400:CO8:H22	3:B:399:FAD:HO2'	1.72	0.54
1:A:251:THR:O	1:A:255:THR:HB	2.07	0.54
1:A:113:ASN:O	1:A:117:GLN:HG3	2.07	0.54
1:B:368:ASP:O	1:B:371:ILE:HG22	2.08	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:45:THR:OG1	1:B:47:GLU:HG3	2.10	0.52
1:B:80:SER:O	1:B:84:THR:HB	2.10	0.52
1:A:203:THR:O	1:A:206:VAL:HG13	2.10	0.51
1:A:252:PHE:O	1:A:256:ARG:HB2	2.11	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
1:B:260:ALA:O	1:B:264:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:178:LEU:C	1:B:178:LEU:HD13	2.37	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:29:LYS:HZ2	1:A:33:GLU:CD	2.22	0.47
1:A:63:ASN:HB3	1:A:66:ILE:CD1	2.45	0.47
1:A:222:THR:C	1:A:223:ARG:HG3	2.39	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:B:255:THR:C	1:B:258:PRO:HD2	2.40	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
1:A:376:GLU:HG2	2:A:400:CO8:H2'2	1.98	0.46
3:A:399:FAD:H51A	1:B:288:LEU:HD21	1.97	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:375:TYR:CD1	1:B:375:TYR:C	2.93	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:A:62:MET:HE3	1:A:101:ASN:ND2	2.32	0.45
1:A:178:LEU:C	1:A:178:LEU:HD13	2.42	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:137:GLU:CD	1:A:149:THR:HG23	2.40	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:333:LYS:NZ	1:B:377:GLY:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:81:CYS:HB3	1:B:312:TYR:CE1	2.52	0.43
1:B:108:LEU:HD23	1:B:121:LEU:CD1	2.37	0.43
1:A:95:GLN:HE21	1:A:95:GLN:HB3	1.61	0.43
1:A:255:THR:HG23	1:A:376:GLU:OE2	2.18	0.43
1:A:255:THR:C	1:A:258:PRO:HD2	2.43	0.43
1:B:103:LEU:HD22	2:B:400:CO8:H5'2	2.00	0.43
1:A:88:ALA:HB1	1:A:92:THR:HG22	2.01	0.43
1:B:63:ASN:ND2	1:B:105:GLN:OE1	2.52	0.43
1:B:181:ARG:NH1	1:B:183:ASP:O	2.46	0.43
1:A:81:CYS:HB3	1:A:312:TYR:CE1	2.53	0.43
1:B:108:LEU:CD1	1:B:198:ILE:HD11	2.41	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: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:B:381:ILE:HD13	1:B:384:ILE:HD12	2.02	0.42
1:B:29:LYS:O	1:B:33:GLU:HB2	2.20	0.42
1:A:354:ASN:HD22	1:B:166:TRP:HZ2	1.67	0.41
1:B:269:ARG:O	1:B:273:GLU:HG2	2.21	0.41
1:A:380:GLN:HE21	1:A:380:GLN:N	2.11	0.41
1:A:267:ALA:HB1	1:A:343:LEU:HD22	2.02	0.41
1:B:63:ASN:HB3	1:B:66:ILE:HD12	2.03	0.41
1:B:181:ARG:NH2	4:B:965:HOH:O	2.53	0.41
1:A:181:ARG:NH2	1:A:185:ASP:O	2.53	0.41
1:A:233:PRO:HB2	1:A:235:GLU:HG2	2.02	0.41
1:B:257:PRO:HB2	1:B:258:PRO:HD3	2.03	0.41
1:B:64:THR:HG23	1:B:75:LEU:CB	2.49	0.41
1:A:378:THR:CG2	3:A:399:FAD:O2B	2.66	0.41
1:B:66:ILE:HA	1:B:67:PRO:HD3	1.90	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
3:A:399:FAD:O3B	1:B:349:GLN:O	2.36	0.41
1:A:120:TYR:CE2	1:A:198:ILE:HG12	2.56	0.41
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.88	0.41
1:A:150:LYS:HD2	1:A:150:LYS:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:310:LEU:HD12	1:B:310:LEU:HA	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

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	383/385 (100%)	377 (98%)	6 (2%)	0	100	100
1	B	383/385 (100%)	376 (98%)	6 (2%)	1 (0%)	36	50
All	All	766/770 (100%)	753 (98%)	12 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/301 (100%)	260 (86%)	41 (14%)	3	5
1	B	301/301 (100%)	267 (89%)	34 (11%)	5	8
All	All	602/602 (100%)	527 (88%)	75 (12%)	4	6

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	64	THR
1	A	75	LEU
1	A	82	LEU
1	A	84	THR
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	149	THR
1	A	156	ASP
1	A	192	LYS
1	A	198	ILE
1	A	206	VAL
1	A	222	THR
1	A	232	VAL
1	A	234	LYS
1	A	235	GLU
1	A	238	LEU
1	A	239	THR
1	A	246	LYS
1	A	255	THR
1	A	256	ARG
1	A	259	VAL
1	A	264	VAL
1	A	266	LEU
1	A	279	LEU
1	A	286	LYS
1	A	288	LEU

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Mol	Chain	Res	Type
1	A	298	LEU
1	A	307	LEU
1	A	310	LEU
1	A	350	VAL
1	A	358	THR
1	A	365	LEU
1	A	375	TYR
1	A	378	THR
1	A	380	GLN
1	B	64	THR
1	B	69	SER
1	B	73	LEU
1	B	82	LEU
1	B	84	THR
1	B	118	LYS
1	B	121	LEU
1	B	129	LEU
1	B	144	VAL
1	B	147	ILE
1	B	153	LYS
1	B	156	ASP
1	B	163	GLN
1	B	192	LYS
1	B	206	VAL
1	B	225	ILE
1	B	234	LYS
1	B	235	GLU
1	B	246	LYS
1	B	255	THR
1	B	256	ARG
1	B	264	VAL
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	310	LEU
1	B	312	TYR
1	B	348	VAL
1	B	358	THR
1	B	365	LEU

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Mol	Chain	Res	Type
1	B	375	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
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
1	A	354	ASN
1	A	373	GLN
1	A	380	GLN
1	A	382	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	217	GLN
1	B	268	GLN
1	B	292	GLN
1	B	313	GLN
1	B	341	ASN
1	B	354	ASN
1	B	373	GLN
1	B	380	GLN
1	B	382	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 oligosaccharides 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	B	399	-	58,58,58	0.98	1 (1%)	85,89,89	1.01	4 (4%)
2	CO8	A	400	-	57,59,59	0.78	1 (1%)	79,85,85	2.21	12 (15%)
2	CO8	B	400	-	57,59,59	0.84	2 (3%)	79,85,85	2.11	13 (16%)
3	FAD	A	399	-	58,58,58	0.96	1 (1%)	85,89,89	1.05	7 (8%)

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	B	399	-	-	0/34/50/50	0/6/6/6
2	CO8	A	400	-	-	15/58/74/74	0/3/3/3
2	CO8	B	400	-	-	14/58/74/74	0/3/3/3
3	FAD	A	399	-	-	1/34/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	399	FAD	C4X-N5	5.09	1.41	1.30
3	A	399	FAD	C4X-N5	4.54	1.40	1.30
2	A	400	CO8	C5P-N4P	2.96	1.40	1.33
2	B	400	CO8	C9P-N8P	2.60	1.39	1.33
2	B	400	CO8	C5P-N4P	2.52	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	CO8	C2'-C1'-S1P	9.01	124.14	113.40
2	A	400	CO8	O1'-C1'-S1P	-8.74	111.57	122.68
2	B	400	CO8	C2'-C1'-S1P	8.24	123.22	113.40
2	B	400	CO8	O1'-C1'-S1P	-7.46	113.19	122.68
2	A	400	CO8	P3B-O3B-C3B	7.31	142.96	123.43
2	A	400	CO8	O6A-CCP-CBP	6.79	121.46	110.55
2	A	400	CO8	C3P-N4P-C5P	-6.30	111.10	122.82
2	B	400	CO8	P3B-O3B-C3B	6.07	139.63	123.43
2	B	400	CO8	O6A-CCP-CBP	5.70	119.71	110.55
2	B	400	CO8	C3P-N4P-C5P	-5.40	112.76	122.82
2	B	400	CO8	C7P-N8P-C9P	-5.31	113.00	122.55
2	B	400	CO8	CAP-C9P-N8P	4.80	125.59	116.48
3	A	399	FAD	C1'-N10-C9A	-4.02	112.81	120.63
2	A	400	CO8	CAP-C9P-N8P	3.72	123.54	116.48
3	B	399	FAD	C1'-N10-C9A	-3.72	113.41	120.63
2	B	400	CO8	O5P-C5P-C6P	-3.43	115.80	122.02
2	B	400	CO8	O9P-C9P-N8P	-3.35	115.90	122.98
3	B	399	FAD	O5'-C5'-C4'	3.30	118.16	109.36
2	A	400	CO8	C7P-N8P-C9P	-3.28	116.66	122.55
2	A	400	CO8	O4B-C1B-N9A	2.95	113.75	108.09
3	A	399	FAD	O4'-C4'-C5'	-2.87	103.65	109.99
2	A	400	CO8	O5P-C5P-C6P	-2.80	116.95	122.02
2	A	400	CO8	C1B-N9A-C8A	2.28	132.16	127.09
3	A	399	FAD	C5X-C9A-N10	-2.28	115.91	117.97
3	B	399	FAD	C10-C4X-N5	-2.26	120.20	124.81
3	A	399	FAD	C5'-C4'-C3'	-2.25	107.97	112.22
2	A	400	CO8	O5A-P2A-O4A	-2.24	102.04	112.44
3	A	399	FAD	C10-C4X-N5	-2.23	120.25	124.81
2	B	400	CO8	C1B-N9A-C8A	2.23	132.05	127.09
3	B	399	FAD	C4-N3-C2	-2.10	121.92	125.64
2	A	400	CO8	O5P-C5P-N4P	2.08	127.10	123.03
2	B	400	CO8	O5A-P2A-O4A	-2.07	102.81	112.44
2	B	400	CO8	CDP-CBP-CCP	-2.05	104.84	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	399	FAD	C10-N1-C2	2.03	121.25	116.85
2	B	400	CO8	O5P-C5P-N4P	2.02	126.99	123.03
3	A	399	FAD	C4X-C10-N1	-2.01	119.67	124.59

There are no chirality outliers.

All (30) torsion outliers are listed below:

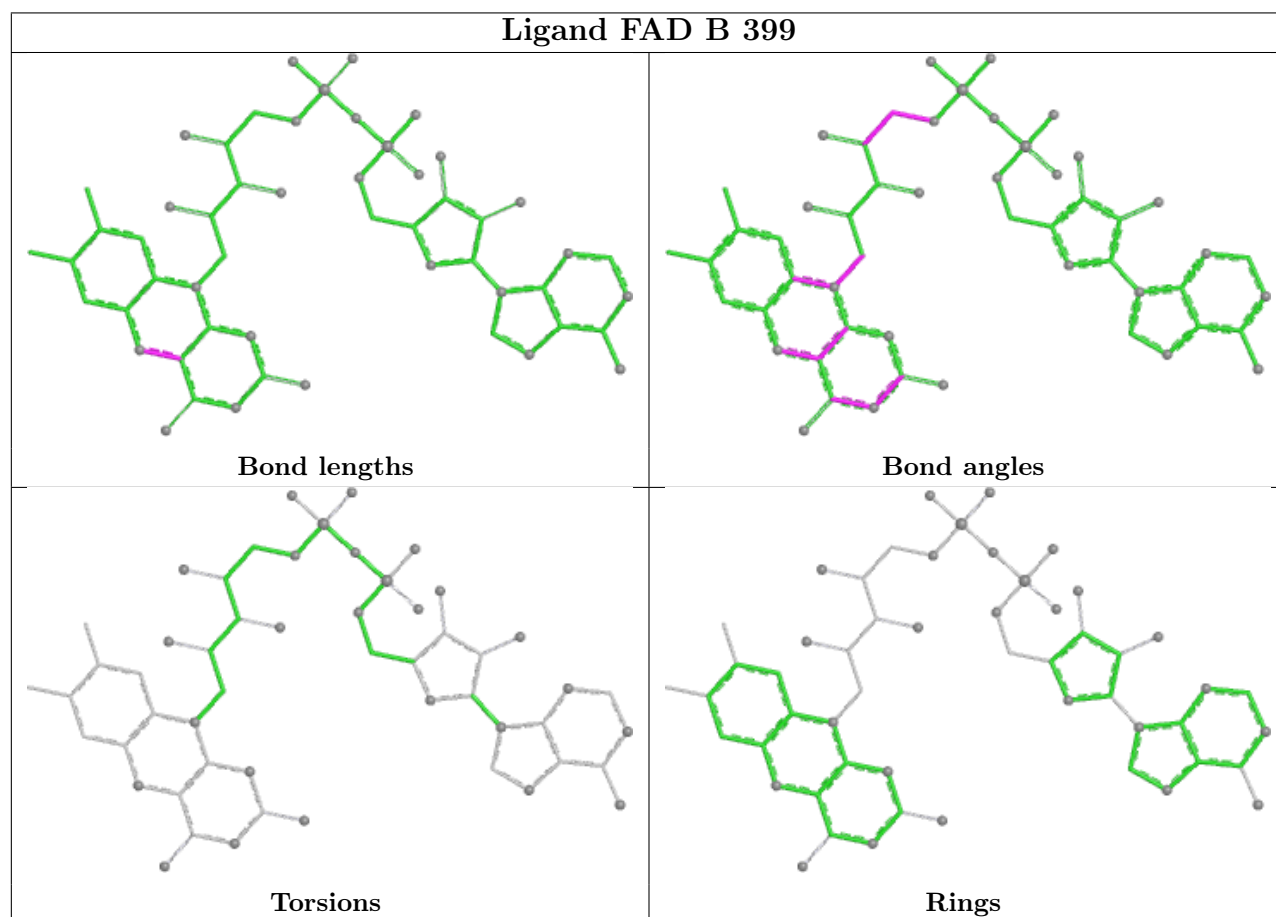
Mol	Chain	Res	Type	Atoms
2	A	400	CO8	CCP-O6A-P2A-O3A
2	A	400	CO8	CCP-O6A-P2A-O4A
2	A	400	CO8	CCP-O6A-P2A-O5A
2	A	400	CO8	C5P-C6P-C7P-N8P
2	A	400	CO8	S1P-C2P-C3P-N4P
2	A	400	CO8	C3P-C2P-S1P-C1'
2	A	400	CO8	C1'-C2'-C3'-C4'
2	B	400	CO8	CCP-O6A-P2A-O5A
2	B	400	CO8	CAP-C9P-N8P-C7P
2	B	400	CO8	C1'-C2'-C3'-C4'
2	B	400	CO8	O9P-C9P-N8P-C7P
2	B	400	CO8	O5P-C5P-N4P-C3P
2	B	400	CO8	C6P-C5P-N4P-C3P
2	B	400	CO8	C5'-C6'-C7'-C8'
2	A	400	CO8	O1'-C1'-S1P-C2P
2	A	400	CO8	C5'-C6'-C7'-C8'
2	A	400	CO8	C2'-C1'-S1P-C2P
2	A	400	CO8	CDP-CBP-CCP-O6A
2	B	400	CO8	CDP-CBP-CCP-O6A
2	B	400	CO8	C3P-C2P-S1P-C1'
2	B	400	CO8	CCP-O6A-P2A-O3A
2	B	400	CO8	CCP-O6A-P2A-O4A
2	A	400	CO8	P1A-O3A-P2A-O4A
2	A	400	CO8	C2'-C3'-C4'-C5'
2	B	400	CO8	P1A-O3A-P2A-O4A
2	B	400	CO8	P1A-O3A-P2A-O5A
3	A	399	FAD	C2'-C3'-C4'-O4'
2	A	400	CO8	C3B-O3B-P3B-O8A
2	A	400	CO8	CEP-CBP-CCP-O6A
2	B	400	CO8	CEP-CBP-CCP-O6A

There are no ring outliers.

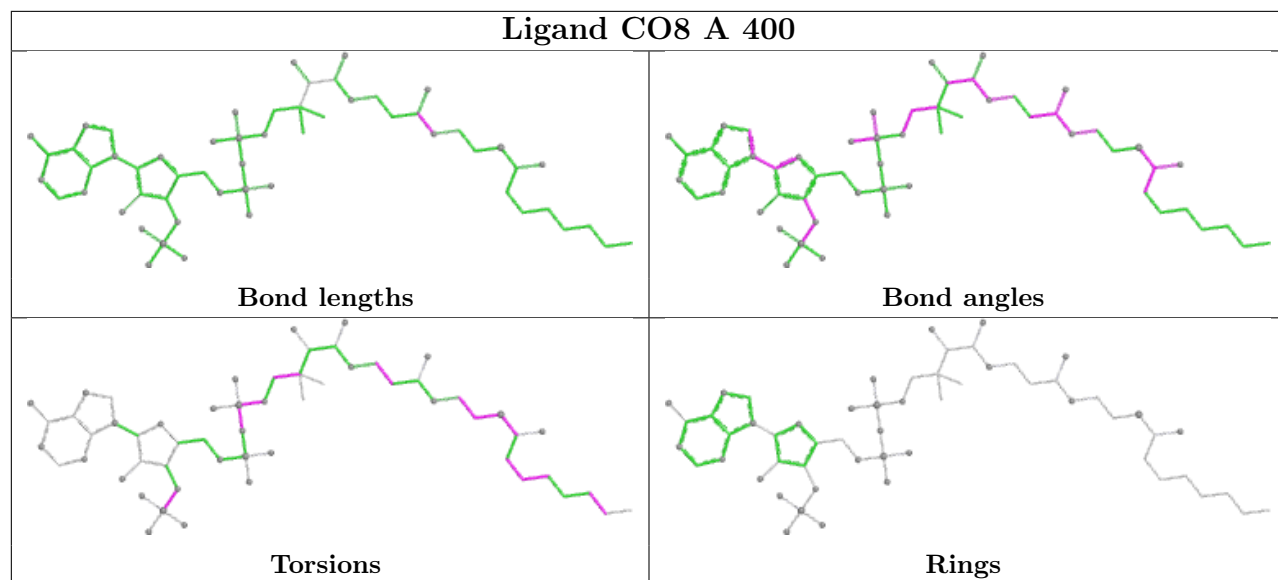
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	399	FAD	2	0
2	A	400	CO8	7	0
2	B	400	CO8	7	0
3	A	399	FAD	5	0

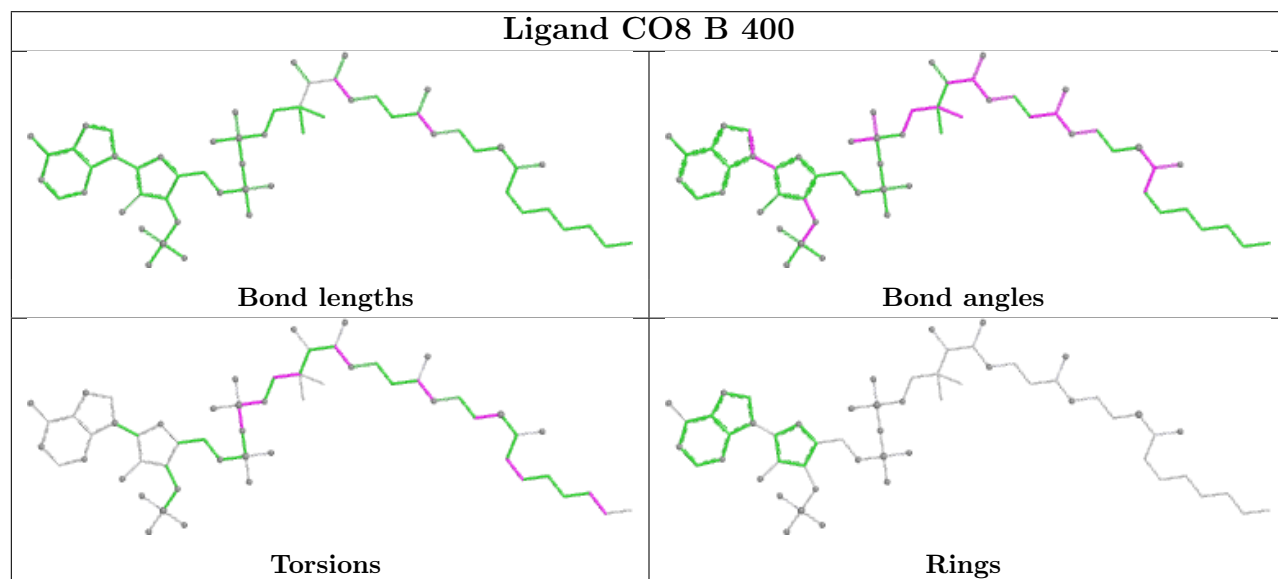
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

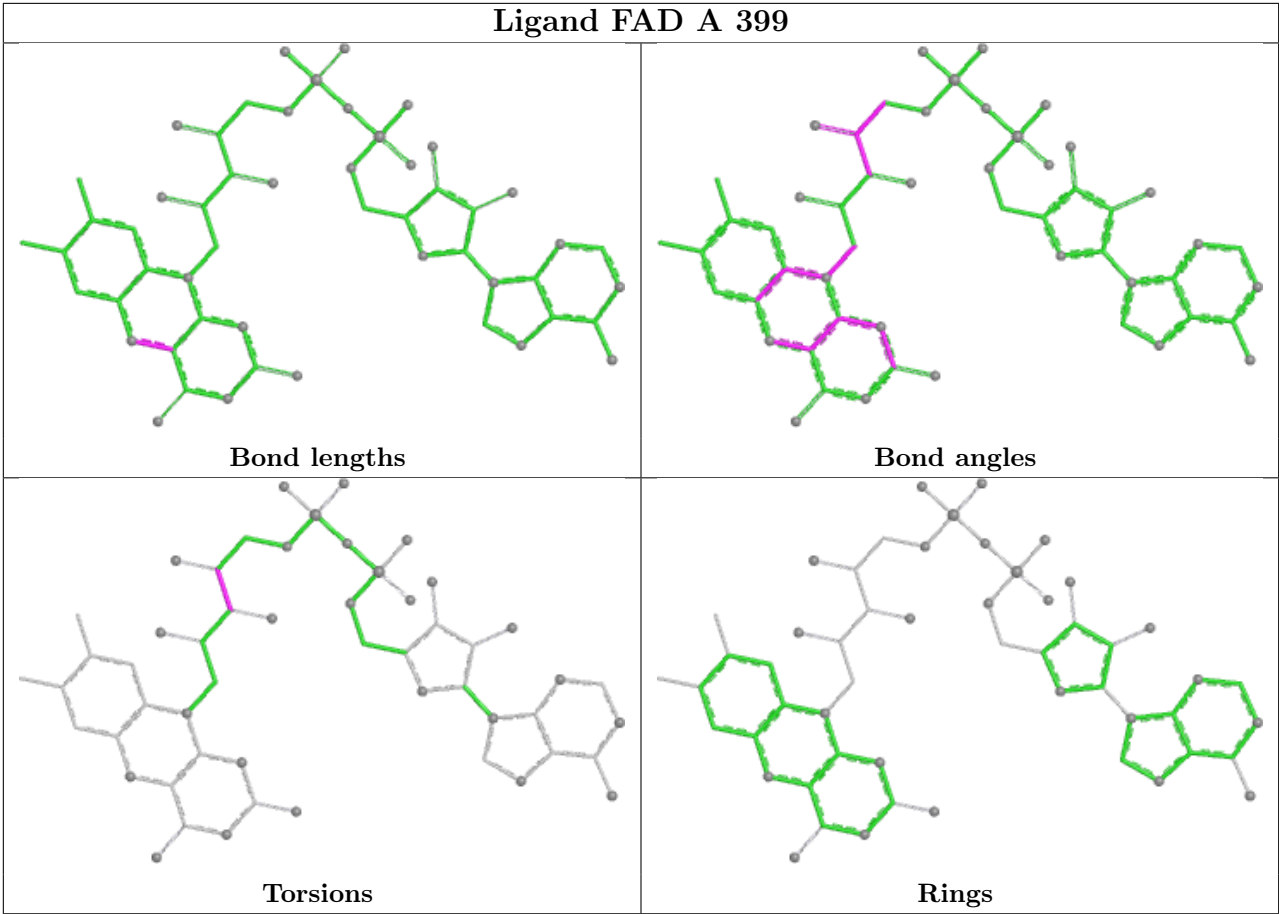


Ligand CO8 A 400



Ligand CO8 B 400





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	377:GLY	C	378:THR	N	1.19

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.