



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:26 AM UTC

PDB ID : 1IS2 / pdb_00001is2
Title : Crystal Structure of Peroxisomal Acyl-CoA Oxidase-II from Rat Liver
Authors : Nakajima, Y.; Miyahara, I.; Hirotsu, K.
Deposited on : 2001-11-07
Resolution : 2.20 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

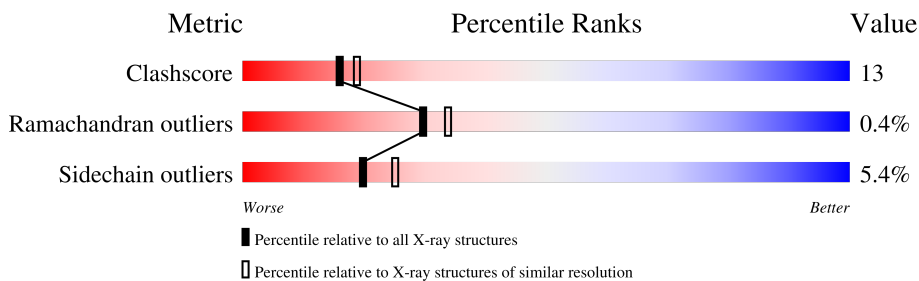
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	661	 72% 21% • •
1	B	661	 65% 26% • 5%

2 Entry composition [i](#)

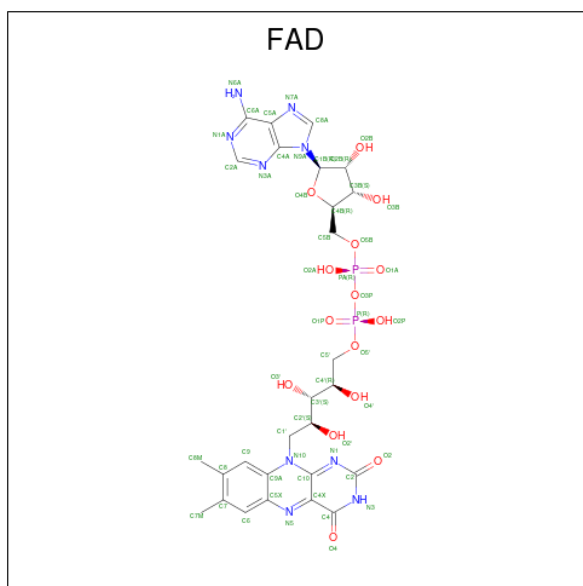
There are 3 unique types of molecules in this entry. The entry contains 10488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	0	0
			5028	3202	867	933	26			
1	B	629	Total	C	N	O	S	0	0	0
			4911	3127	851	909	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is water.

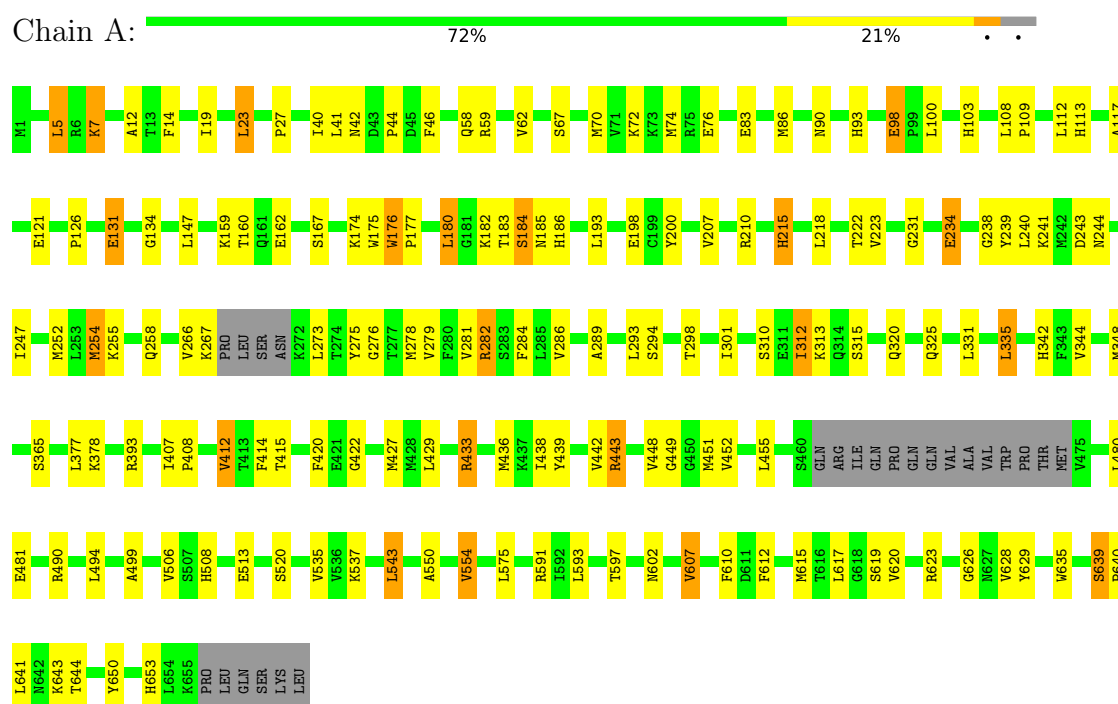
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	241	Total 241	O 241	0	0
3	B	202	Total 202	O 202	0	0

3 Residue-property plots

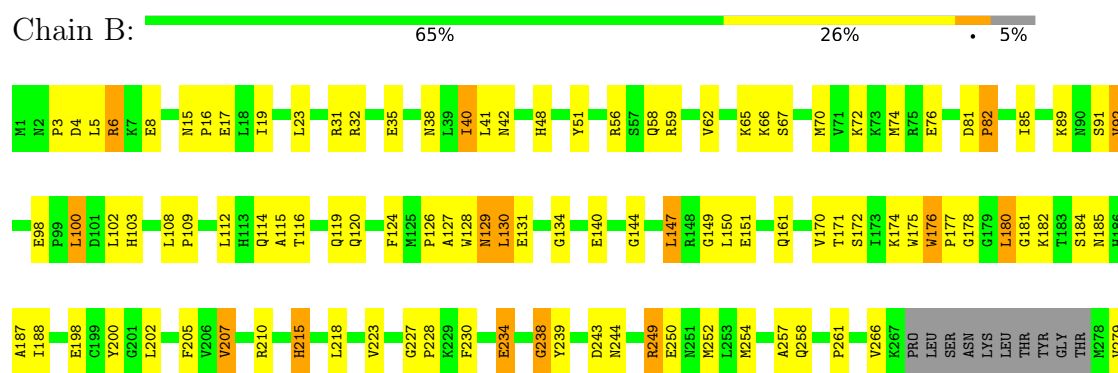
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

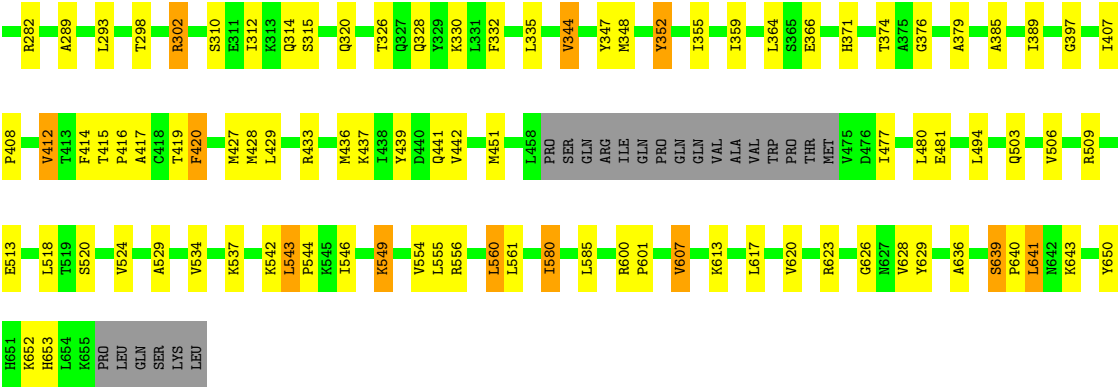
Note EDS was not executed.

• Molecule 1: acyl-CoA oxidase



• Molecule 1: acyl-CoA oxidase





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.03Å 91.50Å 214.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.3 (10.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10488	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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

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	0.46	0/5141	0.94	21/6966 (0.3%)
1	B	0.45	0/5018	0.93	19/6805 (0.3%)
All	All	0.46	0/10159	0.93	40/13771 (0.3%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	VAL	N-CA-C	8.82	118.77	110.74
1	A	628	VAL	N-CA-C	8.63	118.53	110.42
1	A	238	GLY	N-CA-C	7.85	122.56	111.42
1	A	312	ILE	N-CA-C	-7.56	104.49	111.67
1	A	629	TYR	N-CA-C	7.34	119.91	111.11
1	A	98	GLU	CA-C-N	7.31	128.98	119.84
1	A	98	GLU	C-N-CA	7.31	128.98	119.84
1	B	129	ASN	N-CA-C	-6.95	105.61	112.97
1	A	639	SER	CA-C-N	6.84	128.40	119.84
1	A	639	SER	C-N-CA	6.84	128.40	119.84
1	A	131	GLU	N-CA-C	-6.83	103.85	111.71
1	A	331	LEU	N-CA-C	6.69	121.49	113.12
1	B	629	TYR	N-CA-C	6.55	118.97	111.11
1	A	184	SER	N-CA-C	6.23	120.04	110.20
1	B	147	LEU	N-CA-C	5.86	117.67	111.28
1	B	238	GLY	N-CA-C	5.86	119.74	111.42
1	B	98	GLU	CA-C-N	5.79	127.08	119.84
1	B	98	GLU	C-N-CA	5.79	127.08	119.84
1	A	183	THR	N-CA-C	5.64	118.28	111.40
1	A	619	SER	N-CA-C	5.59	118.21	108.76
1	A	275	TYR	N-CA-C	-5.45	105.44	111.71
1	A	415	THR	CA-C-N	-5.39	114.26	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	THR	C-N-CA	-5.39	114.26	119.87
1	B	227	GLY	CA-C-N	5.39	125.29	119.85
1	B	227	GLY	C-N-CA	5.39	125.29	119.85
1	B	310	SER	CB-CA-C	-5.35	109.42	115.79
1	B	639	SER	CA-C-N	5.34	125.41	119.32
1	B	639	SER	C-N-CA	5.34	125.41	119.32
1	A	254	MET	N-CA-C	5.34	119.31	112.26
1	A	520	SER	N-CA-C	5.33	117.09	111.28
1	B	40	ILE	N-CA-C	5.33	116.41	111.45
1	B	320	GLN	N-CA-C	-5.32	102.40	110.28
1	B	184	SER	N-CA-C	5.24	118.23	110.48
1	B	315	SER	N-CA-C	5.24	116.80	111.14
1	A	365	SER	N-CA-C	5.22	116.97	111.28
1	B	266	VAL	N-CA-C	5.11	116.26	108.80
1	B	92	VAL	N-CA-C	5.09	115.70	110.36
1	B	181	GLY	N-CA-C	5.07	118.62	112.49
1	A	167	SER	CA-C-N	5.01	124.79	119.28
1	A	167	SER	C-N-CA	5.01	124.79	119.28

There are no chirality outliers.

There are no planarity outliers.

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	5028	0	4974	118	0
1	B	4911	0	4837	151	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	241	0	0	6	0
3	B	202	0	0	4	0
All	All	10488	0	9873	263	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 13.

All (263) 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:549:LYS:H	1:B:549:LYS:HD3	1.05	1.18
1:B:549:LYS:H	1:B:549:LYS:CD	1.79	0.93
1:B:477:ILE:HD11	1:B:580:ILE:HD11	1.49	0.92
1:A:252:MET:HE2	1:A:254:MET:HG2	1.49	0.91
1:A:273:LEU:HD11	1:A:278:MET:HE3	1.56	0.88
1:B:379:ALA:HB3	1:B:428:MET:HE3	1.59	0.85
1:B:549:LYS:HD3	1:B:549:LYS:N	1.90	0.84
1:B:282:ARG:NE	1:B:427:MET:HE1	1.94	0.83
1:A:103:HIS:HD2	1:A:134:GLY:H	1.27	0.82
1:B:70:MET:HG2	1:B:74:MET:HE2	1.64	0.79
1:B:298:THR:HG23	1:B:607:VAL:HG13	1.65	0.79
1:B:115:ALA:HB3	1:B:120:GLN:HG3	1.66	0.78
1:B:103:HIS:HD2	1:B:134:GLY:H	1.32	0.78
1:A:298:THR:HG23	1:A:607:VAL:HG13	1.65	0.77
1:B:379:ALA:HB3	1:B:428:MET:CE	2.16	0.75
1:A:276:GLY:O	1:A:279:VAL:HG22	1.85	0.75
1:B:282:ARG:CZ	1:B:427:MET:HE1	2.17	0.74
1:A:278:MET:HE2	1:A:278:MET:HA	1.71	0.72
1:A:591:ARG:HH11	1:A:591:ARG:HG2	1.54	0.71
1:A:175:TRP:O	1:A:176:TRP:HB2	1.90	0.71
1:A:70:MET:HG2	1:A:74:MET:HE2	1.72	0.71
1:A:19:ILE:O	1:A:23:LEU:HD22	1.92	0.70
1:A:451:MET:HE2	1:A:451:MET:HA	1.75	0.69
1:B:108:LEU:HB2	1:B:109:PRO:HD3	1.74	0.69
1:A:433:ARG:HG3	1:A:433:ARG:HH11	1.58	0.69
1:A:182:LYS:O	1:A:215:HIS:HE1	1.76	0.68
1:B:494:LEU:HD12	1:B:529:ALA:HB2	1.76	0.68
1:B:175:TRP:O	1:B:176:TRP:HB2	1.92	0.67
1:A:442:VAL:HG13	3:A:1419:HOH:O	1.93	0.67
1:A:160:THR:OG1	1:A:162:GLU:HG2	1.94	0.66
1:A:86:MET:HE3	1:A:90:ASN:HD21	1.61	0.66
1:B:556:ARG:NH1	1:B:560:LEU:HD21	2.09	0.66
1:B:140:GLU:HG2	1:B:174:LYS:HD3	1.78	0.66
1:A:597:THR:HG22	3:A:1385:HOH:O	1.97	0.64
1:A:117:ALA:O	1:A:121:GLU:HG3	1.98	0.64
1:B:636:ALA:O	1:B:639:SER:HB3	1.97	0.64
1:B:477:ILE:HD11	1:B:580:ILE:CD1	2.27	0.63
1:A:451:MET:HE1	1:A:537:LYS:CE	2.28	0.63
1:B:230:PHE:O	1:B:412:VAL:HG21	1.99	0.63
1:A:5:LEU:HD22	1:A:626:GLY:HA3	1.81	0.62
1:A:313:LYS:HE2	1:A:315:SER:OG	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:HG2	1:A:591:ARG:NH1	2.14	0.62
1:B:234:GLU:H	1:B:234:GLU:CD	2.08	0.62
1:B:355:ILE:O	1:B:359:ILE:HG12	2.00	0.61
1:B:72:LYS:O	1:B:76:GLU:HG3	2.01	0.61
1:A:86:MET:HE3	1:A:90:ASN:ND2	2.15	0.60
1:A:234:GLU:CD	1:A:234:GLU:H	2.09	0.60
1:A:162:GLU:HB2	1:A:247:ILE:O	2.03	0.59
1:A:278:MET:O	1:A:281:VAL:HG22	2.03	0.59
1:B:376:GLY:HA2	1:B:428:MET:HE2	1.84	0.58
1:A:480:LEU:HD11	1:A:543:LEU:HD23	1.85	0.58
1:B:279:VAL:HG22	1:B:374:THR:HG21	1.85	0.58
1:A:198:GLU:HB2	1:A:200:TYR:CE1	2.39	0.58
1:B:371:HIS:O	1:B:374:THR:HG22	2.04	0.58
1:B:437:LYS:HE3	1:B:441:GLN:NE2	2.17	0.58
2:B:1699:FAD:O1A	2:B:1699:FAD:H8A	2.04	0.58
1:A:215:HIS:HB2	1:B:650:TYR:CE2	2.39	0.57
1:B:147:LEU:H	1:B:147:LEU:HD12	1.68	0.57
1:B:556:ARG:HH11	1:B:560:LEU:HD21	1.68	0.57
1:B:15:ASN:C	1:B:15:ASN:HD22	2.12	0.56
1:B:51:TYR:OH	1:B:66:LYS:NZ	2.38	0.56
1:A:231:GLY:HA3	1:A:412:VAL:HG13	1.86	0.56
1:A:550:ALA:O	1:A:554:VAL:HG23	2.06	0.56
1:B:556:ARG:NE	3:B:1294:HOH:O	2.39	0.56
1:A:335:LEU:HD23	1:A:335:LEU:O	2.05	0.56
1:A:103:HIS:CD2	1:A:134:GLY:H	2.15	0.56
1:B:40:ILE:CD1	1:B:91:SER:HB2	2.36	0.56
1:B:115:ALA:CB	1:B:120:GLN:HG3	2.33	0.56
1:B:520:SER:O	1:B:524:VAL:HG23	2.05	0.55
1:A:223:VAL:HG12	1:A:240:LEU:HD13	1.88	0.55
1:B:147:LEU:O	1:B:150:LEU:HG	2.06	0.55
1:A:335:LEU:HD23	1:A:335:LEU:C	2.32	0.55
1:A:312:ILE:O	1:B:513:GLU:HG2	2.07	0.55
1:B:126:PRO:C	1:B:128:TRP:H	2.14	0.55
1:A:513:GLU:OE1	1:B:314:GLN:HG2	2.07	0.54
1:B:56:ARG:NH1	3:B:1249:HOH:O	2.40	0.54
1:A:451:MET:HE1	1:A:537:LYS:HE2	1.88	0.54
1:B:67:SER:O	1:B:70:MET:HB3	2.07	0.54
1:B:298:THR:HG23	1:B:607:VAL:CG1	2.36	0.54
1:B:364:LEU:N	1:B:364:LEU:HD12	2.23	0.54
1:B:436:MET:HE2	1:B:436:MET:HA	1.89	0.54
1:A:193:LEU:C	1:A:193:LEU:HD23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MET:CG	1:A:74:MET:HE2	2.38	0.53
1:B:108:LEU:HD21	1:B:127:ALA:CB	2.38	0.53
1:A:513:GLU:HG2	1:B:312:ILE:O	2.09	0.53
1:A:641:LEU:HB2	3:B:1050:HOH:O	2.08	0.53
1:A:174:LYS:O	1:A:239:TYR:HA	2.09	0.52
1:A:67:SER:HB3	1:A:100:LEU:HD12	1.91	0.52
1:B:355:ILE:HD12	1:B:366:GLU:HB2	1.90	0.52
1:A:40:ILE:N	1:A:40:ILE:HD12	2.25	0.52
1:B:126:PRO:O	1:B:131:GLU:HB3	2.10	0.52
1:B:31:ARG:HD3	1:B:31:ARG:C	2.36	0.51
1:B:385:ALA:O	1:B:389:ILE:HG12	2.09	0.51
1:B:414:PHE:C	1:B:416:PRO:HD2	2.35	0.51
1:B:3:PRO:HA	1:B:6:ARG:HG2	1.91	0.51
1:A:348:MET:HE2	1:A:377:LEU:HD12	1.92	0.51
1:A:436:MET:HA	1:A:436:MET:HE2	1.92	0.51
1:B:600:ARG:HB3	1:B:601:PRO:HD3	1.93	0.51
1:A:134:GLY:HA2	1:A:186:HIS:O	2.10	0.51
1:A:310:SER:HB3	3:A:1247:HOH:O	2.11	0.51
1:A:610:PHE:HB3	1:A:612:PHE:CE1	2.46	0.51
1:B:347:TYR:OH	1:B:451:MET:HE2	2.11	0.51
1:A:108:LEU:HB2	1:A:109:PRO:HD3	1.92	0.51
1:A:393:ARG:HB2	1:A:407:ILE:HG21	1.93	0.51
1:A:185:ASN:HA	1:A:210:ARG:HB2	1.93	0.51
1:A:294:SER:OG	1:A:342:HIS:HE1	1.94	0.51
1:A:433:ARG:HH11	1:A:433:ARG:CG	2.23	0.50
1:A:325:GLN:NE2	1:A:593:LEU:HD22	2.27	0.50
1:A:438:ILE:HG23	1:A:448:VAL:HG21	1.94	0.50
1:B:328:GLN:HG2	1:B:332:PHE:CE1	2.46	0.50
1:B:417:ALA:HA	1:B:420:PHE:CE1	2.47	0.50
1:A:103:HIS:HD2	1:A:134:GLY:N	2.04	0.50
1:A:490:ARG:O	1:A:494:LEU:HD23	2.12	0.50
1:A:422:GLY:HA3	1:A:427:MET:HE3	1.94	0.50
1:B:376:GLY:O	1:B:428:MET:HE1	2.10	0.50
1:B:376:GLY:HA2	1:B:428:MET:CE	2.42	0.50
1:B:182:LYS:O	1:B:215:HIS:HE1	1.94	0.50
1:A:620:VAL:O	1:A:623:ARG:HG3	2.11	0.49
1:B:298:THR:O	1:B:302:ARG:HB2	2.12	0.49
1:B:38:ASN:HD21	1:B:613:LYS:HZ1	1.59	0.49
1:B:439:TYR:O	1:B:442:VAL:HG22	2.12	0.49
1:B:38:ASN:HD21	1:B:613:LYS:NZ	2.10	0.49
1:A:298:THR:HG23	1:A:607:VAL:CG1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:HD12	1:B:238:GLY:C	2.37	0.49
1:A:72:LYS:O	1:A:76:GLU:HG3	2.13	0.49
1:A:301:ILE:CD1	1:A:335:LEU:HD12	2.43	0.48
1:A:223:VAL:CG1	1:A:240:LEU:HD13	2.42	0.48
1:A:443:ARG:HG2	1:A:443:ARG:HH11	1.77	0.48
1:B:243:ASP:O	1:B:244:ASN:C	2.56	0.48
1:A:258:GLN:NE2	1:A:267:LYS:HE2	2.28	0.48
1:A:282:ARG:HG3	1:A:282:ARG:NH1	2.27	0.48
1:A:58:GLN:O	1:A:62:VAL:HG23	2.12	0.48
1:B:32:ARG:NH1	1:B:35:GLU:OE2	2.46	0.48
1:A:14:PHE:CD2	1:A:554:VAL:HG21	2.48	0.48
1:B:40:ILE:HD13	1:B:91:SER:HB2	1.96	0.48
1:B:289:ALA:HA	1:B:414:PHE:CE2	2.48	0.48
1:B:129:ASN:C	1:B:131:GLU:N	2.72	0.48
1:B:252:MET:HE2	1:B:254:MET:HG2	1.94	0.48
1:B:437:LYS:HE3	1:B:441:GLN:HE22	1.76	0.48
1:B:509:ARG:NH1	1:B:518:LEU:HD11	2.29	0.48
1:A:282:ARG:HG3	1:A:282:ARG:HH11	1.79	0.47
1:A:93:HIS:CD2	1:A:98:GLU:HG2	2.49	0.47
1:B:147:LEU:C	1:B:149:GLY:H	2.20	0.47
1:B:543:LEU:HB2	1:B:544:PRO:HD3	1.95	0.47
1:A:643:LYS:HG3	1:A:644:THR:HG23	1.95	0.47
1:B:15:ASN:C	1:B:15:ASN:ND2	2.71	0.47
1:B:103:HIS:CD2	1:B:134:GLY:H	2.20	0.47
1:B:112:LEU:C	1:B:112:LEU:HD13	2.39	0.47
1:A:289:ALA:HA	1:A:414:PHE:CE2	2.49	0.47
1:A:12:ALA:HA	1:A:602:ASN:OD1	2.15	0.47
1:A:19:ILE:HG22	1:A:23:LEU:CD2	2.44	0.47
1:A:40:ILE:HG23	1:A:46:PHE:CD1	2.48	0.47
1:A:480:LEU:HD11	1:A:543:LEU:CD2	2.44	0.47
1:B:15:ASN:HD22	1:B:16:PRO:N	2.13	0.47
1:B:112:LEU:HD13	1:B:112:LEU:O	2.15	0.47
1:B:187:ALA:O	1:B:207:VAL:HG13	2.15	0.47
1:B:376:GLY:O	1:B:428:MET:CE	2.63	0.47
1:A:243:ASP:O	1:A:244:ASN:C	2.58	0.46
1:B:51:TYR:HB3	1:B:59:ARG:HD3	1.95	0.46
1:B:451:MET:SD	1:B:537:LYS:HD3	2.55	0.46
1:A:103:HIS:HE1	3:A:1093:HOH:O	1.97	0.46
1:A:126:PRO:HB3	1:A:131:GLU:OE1	2.15	0.46
1:A:635:TRP:CH2	1:B:228:PRO:HD2	2.51	0.46
1:B:176:TRP:O	1:B:177:PRO:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:O	1:B:348:MET:HG3	2.15	0.46
1:A:5:LEU:HD22	1:A:626:GLY:CA	2.45	0.46
1:A:438:ILE:CG2	1:A:448:VAL:HG21	2.46	0.46
1:B:185:ASN:HA	1:B:210:ARG:HB2	1.98	0.46
1:B:198:GLU:HB3	1:B:200:TYR:CE1	2.51	0.46
1:B:481:GLU:H	1:B:481:GLU:CD	2.23	0.46
1:B:41:LEU:C	1:B:41:LEU:HD13	2.40	0.46
1:B:546:ILE:HD13	1:B:555:LEU:HD12	1.97	0.46
1:A:86:MET:CE	1:A:90:ASN:HD21	2.27	0.46
1:A:298:THR:HA	1:A:607:VAL:CG1	2.46	0.45
1:A:650:TYR:CE2	1:B:215:HIS:HB2	2.51	0.45
1:B:174:LYS:O	1:B:239:TYR:HA	2.16	0.45
1:A:222:THR:HB	1:A:241:LYS:HB3	1.97	0.45
1:A:175:TRP:O	1:A:176:TRP:CB	2.61	0.45
1:A:126:PRO:O	1:A:131:GLU:HB3	2.15	0.45
1:A:286:VAL:HG23	3:A:1421:HOH:O	2.16	0.45
1:B:40:ILE:HD12	1:B:91:SER:HB2	1.98	0.45
1:B:112:LEU:HB2	1:B:124:PHE:CE1	2.52	0.45
1:B:302:ARG:NH2	3:B:1005:HOH:O	2.41	0.45
1:B:15:ASN:HD22	1:B:16:PRO:CD	2.30	0.45
1:B:250:GLU:CD	1:B:250:GLU:H	2.24	0.45
1:A:639:SER:HB2	1:A:640:PRO:HD2	1.99	0.45
1:A:273:LEU:CD1	1:A:278:MET:HE3	2.37	0.45
1:A:344:VAL:HG21	1:A:535:VAL:HG22	1.98	0.45
1:B:15:ASN:ND2	1:B:17:GLU:H	2.14	0.45
1:B:115:ALA:HB3	1:B:120:GLN:CG	2.43	0.45
1:A:506:VAL:C	1:A:508:HIS:H	2.25	0.44
1:A:653:HIS:CE1	1:B:65:LYS:HD2	2.52	0.44
1:B:407:ILE:N	1:B:408:PRO:CD	2.81	0.44
1:B:58:GLN:O	1:B:62:VAL:HG23	2.17	0.44
1:B:67:SER:HB3	1:B:100:LEU:HD22	1.98	0.44
1:B:451:MET:HG2	1:B:534:VAL:HG22	1.98	0.44
1:A:113:HIS:O	1:A:255:LYS:HE3	2.17	0.44
1:B:477:ILE:HD13	1:B:477:ILE:HA	1.80	0.44
1:B:640:PRO:O	1:B:643:LYS:HG2	2.17	0.44
1:A:448:VAL:HG22	1:A:449:GLY:N	2.33	0.43
1:B:254:MET:HB3	1:B:258:GLN:HG3	2.00	0.43
1:B:38:ASN:ND2	1:B:613:LYS:NZ	2.67	0.43
1:B:175:TRP:C	1:B:177:PRO:HD3	2.43	0.43
1:B:128:TRP:C	1:B:130:LEU:H	2.24	0.43
1:A:408:PRO:O	1:A:412:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:TYR:CE2	1:A:499:ALA:HB1	2.53	0.43
1:B:249:ARG:NH1	1:B:250:GLU:OE2	2.52	0.43
1:A:27:PRO:HD2	3:A:1354:HOH:O	2.18	0.43
1:A:481:GLU:OE2	1:A:481:GLU:N	2.52	0.43
1:B:202:LEU:N	1:B:202:LEU:HD22	2.34	0.43
1:B:5:LEU:HD12	1:B:626:GLY:HA3	2.01	0.43
1:B:352:TYR:C	1:B:352:TYR:CD2	2.97	0.43
1:B:620:VAL:O	1:B:623:ARG:HG3	2.19	0.43
1:B:126:PRO:C	1:B:128:TRP:N	2.77	0.43
1:B:102:LEU:HD12	1:B:178:GLY:O	2.19	0.42
1:B:108:LEU:HD21	1:B:127:ALA:HB3	2.00	0.42
1:B:542:LYS:O	1:B:542:LYS:HD3	2.19	0.42
1:B:641:LEU:HD12	1:B:641:LEU:HA	1.87	0.42
1:A:42:ASN:O	1:A:44:PRO:HD3	2.18	0.42
1:B:4:ASP:O	1:B:8:GLU:HG2	2.20	0.42
1:B:161:GLN:NE2	1:B:261:PRO:HB3	2.33	0.42
1:A:282:ARG:HD2	1:A:284:PHE:CZ	2.54	0.42
1:A:451:MET:HE1	1:A:537:LYS:HD3	2.02	0.42
1:A:480:LEU:CD1	1:A:543:LEU:HD23	2.48	0.42
1:B:151:GLU:HB2	1:B:172:SER:CB	2.49	0.42
1:B:282:ARG:HH11	1:B:374:THR:HG23	1.84	0.42
1:A:258:GLN:HB2	1:A:266:VAL:CG2	2.50	0.42
1:B:234:GLU:CD	1:B:234:GLU:N	2.77	0.42
1:B:175:TRP:O	1:B:177:PRO:HD3	2.19	0.42
1:B:652:LYS:HG3	1:B:653:HIS:CD2	2.54	0.42
1:A:451:MET:HE1	1:A:537:LYS:CD	2.50	0.42
1:B:250:GLU:CD	1:B:250:GLU:N	2.78	0.42
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.86	0.42
1:A:177:PRO:HB2	1:A:180:LEU:HB2	2.02	0.42
1:A:452:VAL:HG22	1:A:455:LEU:HD12	2.01	0.42
1:B:170:VAL:HG13	1:B:171:THR:N	2.35	0.42
1:A:7:LYS:HZ3	1:A:320:GLN:HE22	1.67	0.42
1:B:481:GLU:CD	1:B:481:GLU:N	2.78	0.42
1:A:258:GLN:HB2	1:A:266:VAL:HG22	2.02	0.41
1:B:82:PRO:HA	1:B:85:ILE:HD12	2.01	0.41
1:A:67:SER:O	1:A:70:MET:HB3	2.19	0.41
1:A:175:TRP:C	1:A:177:PRO:HD3	2.45	0.41
1:A:40:ILE:HD12	1:A:40:ILE:H	1.85	0.41
1:A:184:SER:O	1:A:210:ARG:HD2	2.20	0.41
1:B:298:THR:HA	1:B:607:VAL:CG1	2.50	0.41
1:B:48:HIS:CE1	1:B:66:LYS:HZ2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASP:HA	1:B:82:PRO:HD2	1.91	0.41
2:A:699:FAD:H51A	1:B:397:GLY:HA3	2.03	0.41
1:B:19:ILE:O	1:B:23:LEU:HG	2.21	0.41
1:B:66:LYS:HE3	1:B:92:VAL:O	2.21	0.41
1:B:147:LEU:C	1:B:149:GLY:N	2.78	0.41
1:B:89:LYS:HD3	1:B:89:LYS:C	2.45	0.41
1:B:175:TRP:O	1:B:176:TRP:CB	2.64	0.41
1:B:503:GLN:HA	1:B:506:VAL:HG22	2.01	0.41
1:A:452:VAL:HG22	1:A:455:LEU:CD1	2.51	0.40
1:B:188:ILE:HA	1:B:205:PHE:O	2.21	0.40
1:B:254:MET:HA	1:B:257:ALA:O	2.20	0.40
1:A:378:LYS:CE	1:A:420:PHE:O	2.69	0.40
1:B:41:LEU:HD12	1:B:42:ASN:OD1	2.22	0.40
1:B:415:THR:N	1:B:416:PRO:HD2	2.36	0.40
1:B:116:THR:OG1	1:B:119:GLN:HG3	2.21	0.40
1:B:639:SER:HA	1:B:640:PRO:HD3	1.92	0.40
1:B:326:THR:O	1:B:330:LYS:HG3	2.22	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	631/661 (96%)	615 (98%)	15 (2%)	1 (0%)	43	51
1	B	623/661 (94%)	597 (96%)	22 (4%)	4 (1%)	21	23
All	All	1254/1322 (95%)	1212 (97%)	37 (3%)	5 (0%)	30	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP

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Mol	Chain	Res	Type
1	B	176	TRP
1	B	114	GLN
1	B	82	PRO
1	B	144	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	539/571 (94%)	512 (95%)	27 (5%)	22	28
1	B	519/571 (91%)	489 (94%)	30 (6%)	18	22
All	All	1058/1142 (93%)	1001 (95%)	57 (5%)	20	25

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	LYS
1	A	23	LEU
1	A	41	LEU
1	A	59	ARG
1	A	83	GLU
1	A	112	LEU
1	A	147	LEU
1	A	159	LYS
1	A	180	LEU
1	A	207	VAL
1	A	215	HIS
1	A	218	LEU
1	A	234	GLU
1	A	282	ARG
1	A	293	LEU
1	A	335	LEU
1	A	412	VAL
1	A	429	LEU

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Mol	Chain	Res	Type
1	A	433	ARG
1	A	443	ARG
1	A	543	LEU
1	A	554	VAL
1	A	575	LEU
1	A	607	VAL
1	A	615	MET
1	A	617	LEU
1	B	6	ARG
1	B	100	LEU
1	B	130	LEU
1	B	180	LEU
1	B	207	VAL
1	B	215	HIS
1	B	218	LEU
1	B	223	VAL
1	B	234	GLU
1	B	249	ARG
1	B	293	LEU
1	B	302	ARG
1	B	335	LEU
1	B	344	VAL
1	B	352	TYR
1	B	412	VAL
1	B	419	THR
1	B	420	PHE
1	B	429	LEU
1	B	433	ARG
1	B	480	LEU
1	B	543	LEU
1	B	549	LYS
1	B	554	VAL
1	B	560	LEU
1	B	561	LEU
1	B	580	ILE
1	B	585	LEU
1	B	607	VAL
1	B	641	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	38	ASN
1	A	47	GLN
1	A	48	HIS
1	A	90	ASN
1	A	103	HIS
1	A	113	HIS
1	A	114	GLN
1	A	203	HIS
1	A	215	HIS
1	A	258	GLN
1	A	291	GLN
1	A	320	GLN
1	A	386	ASN
1	A	409	ASN
1	A	503	GLN
1	A	557	ASN
1	A	587	GLN
1	A	627	ASN
1	A	647	HIS
1	A	653	HIS
1	B	15	ASN
1	B	21	HIS
1	B	38	ASN
1	B	48	HIS
1	B	93	HIS
1	B	103	HIS
1	B	138	GLN
1	B	161	GLN
1	B	203	HIS
1	B	215	HIS
1	B	361	GLN
1	B	371	HIS
1	B	430	GLN
1	B	441	GLN
1	B	557	ASN
1	B	589	ASN
1	B	627	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
2	FAD	B	1699	-	58,58,58	2.34	17 (29%)	85,89,89	1.10	7 (8%)
2	FAD	A	699	-	58,58,58	2.33	16 (27%)	85,89,89	1.15	6 (7%)

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
2	FAD	B	1699	-	-	4/34/50/50	0/6/6/6
2	FAD	A	699	-	-	4/34/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	699	FAD	P-O3P	-12.04	1.46	1.59
2	B	1699	FAD	P-O3P	-11.98	1.46	1.59
2	A	699	FAD	PA-O2A	-4.31	1.35	1.55
2	B	1699	FAD	PA-O2A	-4.26	1.35	1.55
2	A	699	FAD	O5'-C5'	4.21	1.60	1.44
2	B	1699	FAD	O5'-C5'	3.89	1.59	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1699	FAD	P-O2P	-3.74	1.38	1.55
2	A	699	FAD	P-O2P	-3.69	1.38	1.55
2	B	1699	FAD	C9A-N10	3.37	1.47	1.41
2	B	1699	FAD	C1'-C2'	3.20	1.57	1.52
2	A	699	FAD	C8-C7	2.99	1.48	1.40
2	A	699	FAD	O4B-C1B	2.98	1.48	1.42
2	B	1699	FAD	C8-C7	2.91	1.48	1.40
2	A	699	FAD	C9A-C5X	2.80	1.45	1.41
2	B	1699	FAD	O4B-C1B	2.77	1.48	1.42
2	A	699	FAD	C5A-C6A	2.77	1.48	1.41
2	A	699	FAD	C9A-N10	2.72	1.45	1.41
2	B	1699	FAD	C9A-C5X	2.48	1.45	1.41
2	A	699	FAD	O2-C2	-2.43	1.19	1.24
2	A	699	FAD	C4X-N5	2.34	1.35	1.30
2	B	1699	FAD	C5A-C6A	2.32	1.47	1.41
2	B	1699	FAD	O2-C2	-2.27	1.19	1.24
2	B	1699	FAD	C4A-N3A	2.26	1.38	1.34
2	B	1699	FAD	C2-N3	2.25	1.43	1.39
2	B	1699	FAD	C5A-C4A	2.19	1.43	1.39
2	B	1699	FAD	O4B-C4B	2.18	1.49	1.45
2	B	1699	FAD	C4X-N5	2.17	1.35	1.30
2	A	699	FAD	C2-N3	2.10	1.43	1.39
2	A	699	FAD	C5A-C4A	2.09	1.42	1.39
2	A	699	FAD	C4A-N3A	2.08	1.38	1.34
2	A	699	FAD	C1'-C2'	2.07	1.55	1.52
2	A	699	FAD	O4B-C4B	2.06	1.49	1.45
2	B	1699	FAD	C10-N1	2.06	1.37	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	699	FAD	O5B-PA-O1A	-3.02	96.97	108.94
2	A	699	FAD	O2A-PA-O3P	2.94	115.23	107.27
2	B	1699	FAD	O5B-PA-O1A	-2.77	97.97	108.94
2	B	1699	FAD	C2A-N1A-C6A	2.71	123.17	118.73
2	A	699	FAD	C2A-N1A-C6A	2.66	123.10	118.73
2	A	699	FAD	O3B-C3B-C4B	2.61	118.58	111.08
2	B	1699	FAD	C5X-C9A-N10	-2.33	115.86	117.97
2	B	1699	FAD	O2A-PA-O3P	2.25	113.37	107.27
2	B	1699	FAD	C4-N3-C2	-2.23	121.69	125.64
2	B	1699	FAD	O3B-C3B-C4B	2.20	117.39	111.08
2	A	699	FAD	C4-N3-C2	-2.19	121.76	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	699	FAD	C5X-C9A-N10	-2.14	116.03	117.97
2	B	1699	FAD	C4X-C10-N10	2.04	119.41	116.48

There are no chirality outliers.

All (8) torsion outliers are listed below:

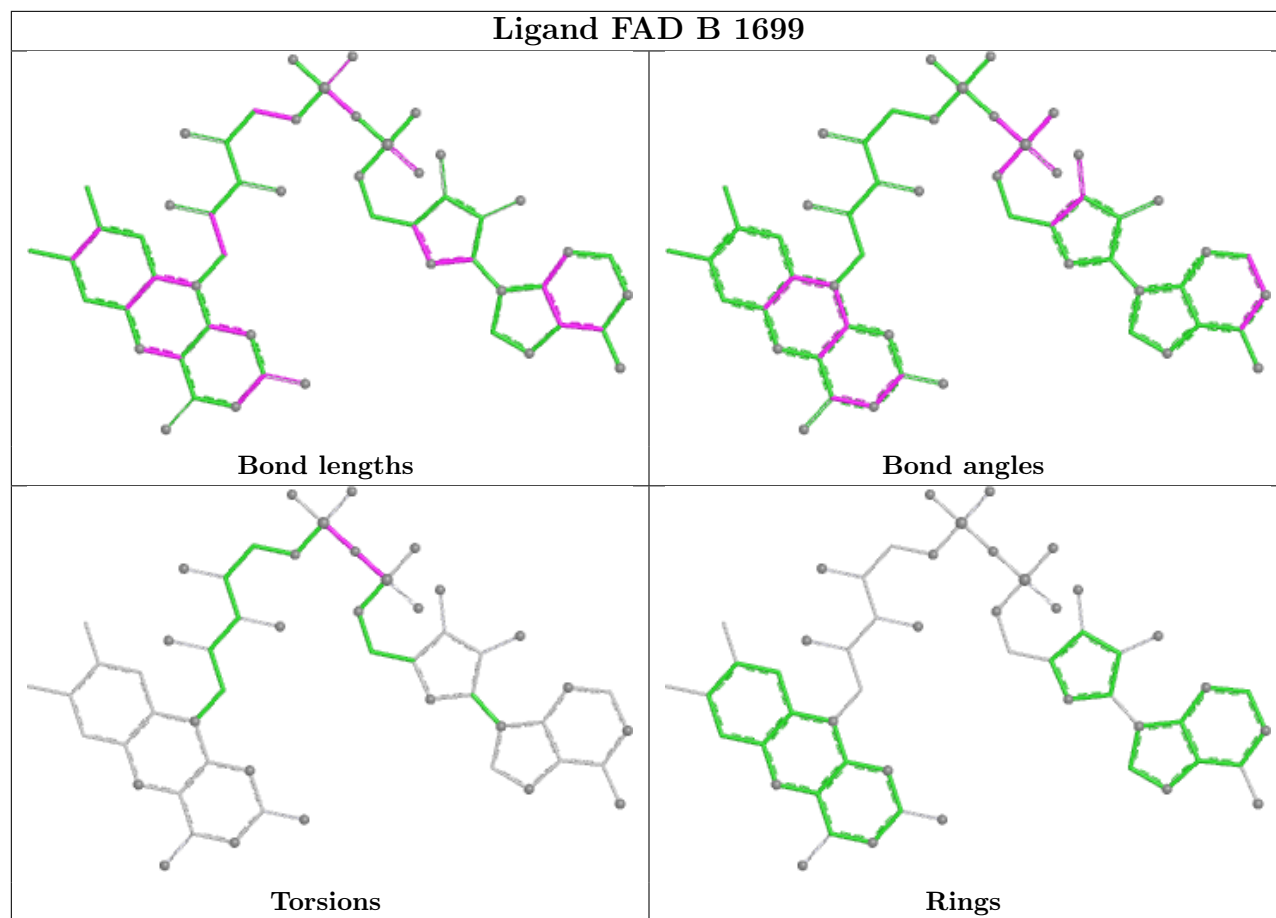
Mol	Chain	Res	Type	Atoms
2	A	699	FAD	P-O3P-PA-O2A
2	A	699	FAD	PA-O3P-P-O2P
2	B	1699	FAD	P-O3P-PA-O2A
2	A	699	FAD	P-O3P-PA-O1A
2	B	1699	FAD	PA-O3P-P-O2P
2	A	699	FAD	PA-O3P-P-O1P
2	B	1699	FAD	PA-O3P-P-O1P
2	B	1699	FAD	P-O3P-PA-O1A

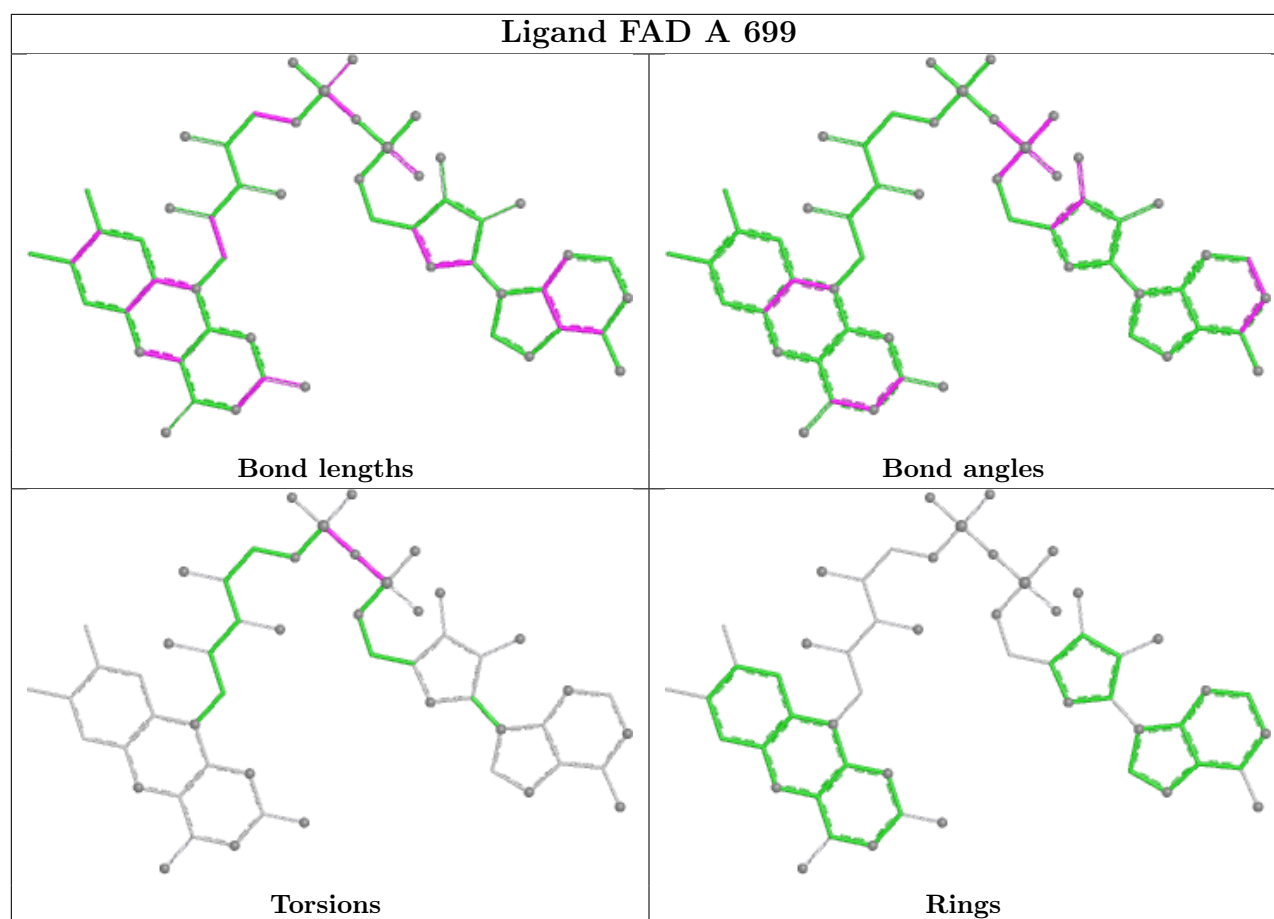
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1699	FAD	1	0
2	A	699	FAD	1	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.