Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 09:36 PM JST

PDB ID	:	5Y9D
Title	:	Crystal structure of acyl-coA oxidase1 from Yarrowia lipolytica
Authors	:	Kim, S.; Kim, K.-J.
Deposited on	:	2017-08-24
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

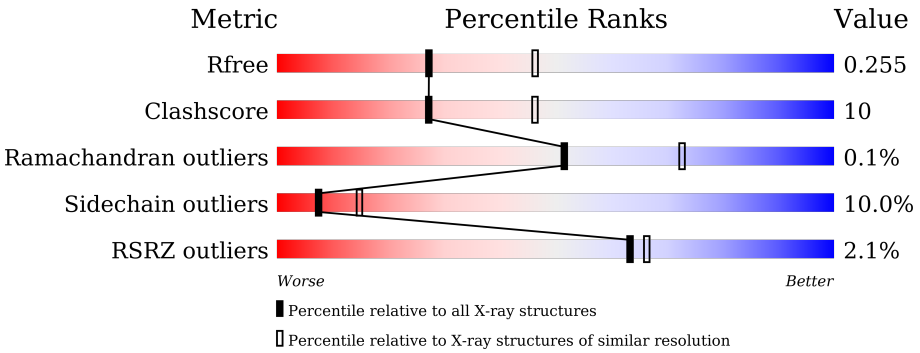
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

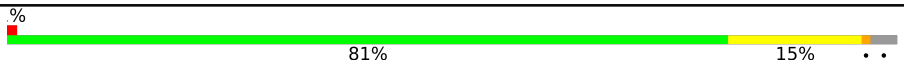
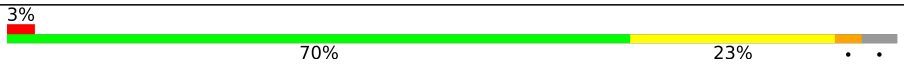
The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	709	
1	B	709	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10952 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-coenzyme A oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5418	3417	948	1025	28			
1	B	682	Total	C	N	O	S	0	0	0
			5382	3394	942	1018	28			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O74934
A	-18	GLY	-	expression tag	UNP O74934
A	-17	SER	-	expression tag	UNP O74934
A	-16	SER	-	expression tag	UNP O74934
A	-15	HIS	-	expression tag	UNP O74934
A	-14	HIS	-	expression tag	UNP O74934
A	-13	HIS	-	expression tag	UNP O74934
A	-12	HIS	-	expression tag	UNP O74934
A	-11	HIS	-	expression tag	UNP O74934
A	-10	HIS	-	expression tag	UNP O74934
A	-9	SER	-	expression tag	UNP O74934
A	-8	SER	-	expression tag	UNP O74934
A	-7	GLY	-	expression tag	UNP O74934
A	-6	LEU	-	expression tag	UNP O74934
A	-5	VAL	-	expression tag	UNP O74934
A	-4	PRO	-	expression tag	UNP O74934
A	-3	ARG	-	expression tag	UNP O74934
A	-2	GLY	-	expression tag	UNP O74934
A	-1	SER	-	expression tag	UNP O74934
A	0	HIS	-	expression tag	UNP O74934
B	-19	MET	-	expression tag	UNP O74934
B	-18	GLY	-	expression tag	UNP O74934
B	-17	SER	-	expression tag	UNP O74934
B	-16	SER	-	expression tag	UNP O74934
B	-15	HIS	-	expression tag	UNP O74934

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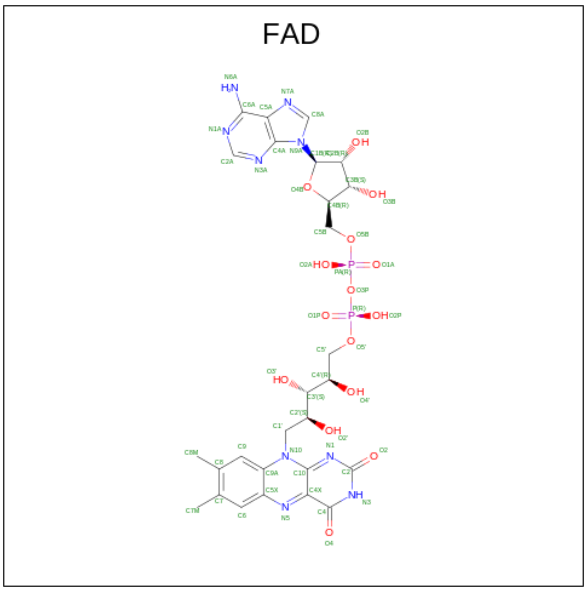
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP O74934
B	-13	HIS	-	expression tag	UNP O74934
B	-12	HIS	-	expression tag	UNP O74934
B	-11	HIS	-	expression tag	UNP O74934
B	-10	HIS	-	expression tag	UNP O74934
B	-9	SER	-	expression tag	UNP O74934
B	-8	SER	-	expression tag	UNP O74934
B	-7	GLY	-	expression tag	UNP O74934
B	-6	LEU	-	expression tag	UNP O74934
B	-5	VAL	-	expression tag	UNP O74934
B	-4	PRO	-	expression tag	UNP O74934
B	-3	ARG	-	expression tag	UNP O74934
B	-2	GLY	-	expression tag	UNP O74934
B	-1	SER	-	expression tag	UNP O74934
B	0	HIS	-	expression tag	UNP O74934

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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.

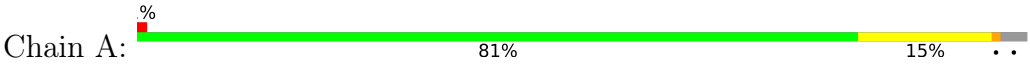
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	25	Total O 25 25	0	0
3	B	21	Total O 21 21	0	0

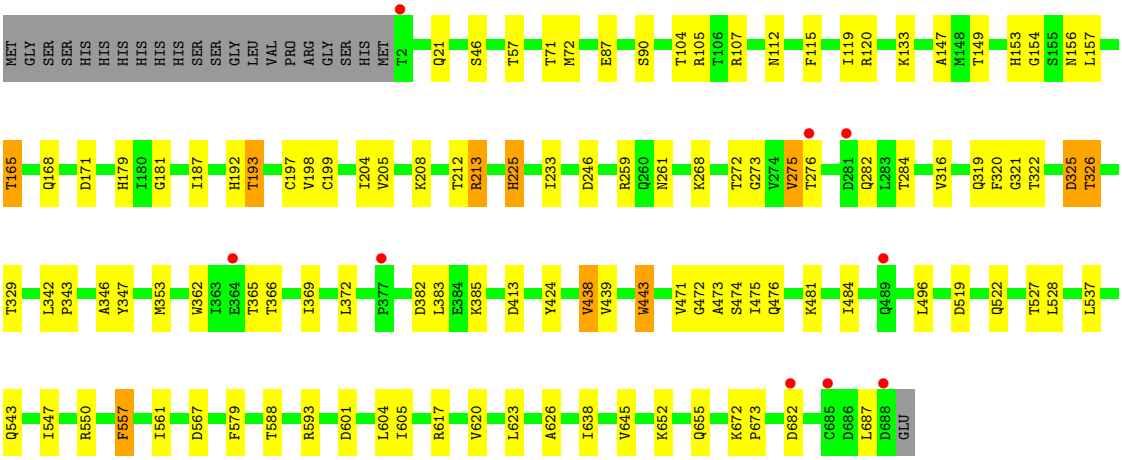
3 Residue-property plots (i)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Acyl-coenzyme A oxidase 1

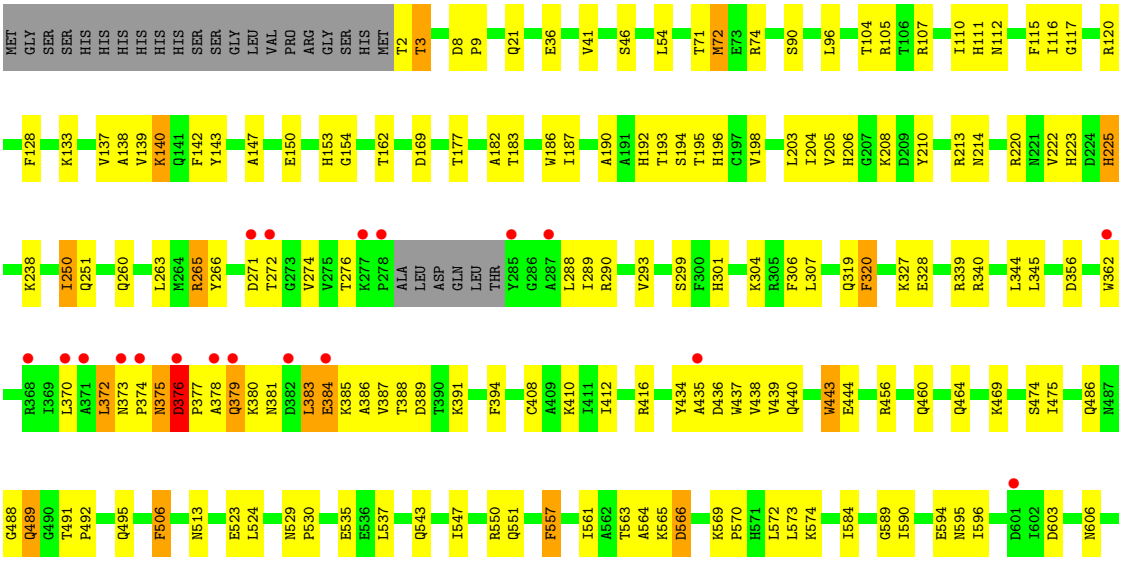
Chain A:

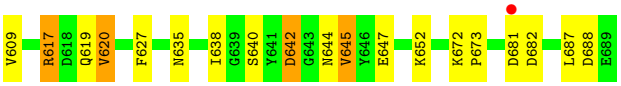




• Molecule 1: Acyl-coenzyme A oxidase 1

Chain B:




V609
R617
D618
Q619
V620
F627
N635
I638
G639
S640
Y641
D642
G643
N644
V645
Y646
E647
K652
K672
P673
D681
D682
L687
D688
E689

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	167.88Å 167.88Å 95.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.95 – 2.50 32.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.95-2.50) 99.1 (32.92-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.21 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.183 , 0.253 0.184 , 0.255	Depositor DCC
R_{free} test set	2182 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 18.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.074 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10952	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.62	0/5531	0.75	0/7490
1	B	0.58	0/5494	0.72	1/7437 (0.0%)
All	All	0.60	0/11025	0.74	1/14927 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	320	PHE	N-CA-C	5.19	125.02	111.00

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	5418	0	5340	71	0
1	B	5382	0	5299	154	0
2	A	53	0	31	9	0
2	B	53	0	31	13	0
3	A	25	0	0	0	0
3	B	21	0	0	1	0
All	All	10952	0	10701	219	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 10.

All (219) 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:373:ASN:HD22	1:B:376:ASP:CB	1.08	1.57
1:B:373:ASN:ND2	1:B:376:ASP:HB2	1.30	1.39
1:B:373:ASN:ND2	1:B:376:ASP:CB	1.79	1.38
1:B:373:ASN:HB3	1:B:376:ASP:CB	1.64	1.27
1:B:373:ASN:HD22	1:B:376:ASP:CG	1.39	1.26
1:B:373:ASN:CB	1:B:376:ASP:HB3	1.74	1.17
1:B:373:ASN:CB	1:B:376:ASP:CB	2.25	1.14
1:B:373:ASN:ND2	1:B:376:ASP:CG	2.01	1.05
1:B:373:ASN:CG	1:B:376:ASP:HB2	1.80	1.00
1:B:372:LEU:CD2	1:B:383:LEU:HD22	1.91	1.00
1:B:373:ASN:CG	1:B:376:ASP:CB	2.34	0.95
1:B:564:ALA:O	1:B:569:LYS:HD2	1.68	0.94
1:B:373:ASN:HB3	1:B:376:ASP:HB3	1.35	0.94
1:B:439:VAL:HG23	2:B:701:FAD:HM83	1.55	0.89
1:B:372:LEU:HD23	1:B:383:LEU:HD22	1.51	0.89
1:B:373:ASN:HD22	1:B:376:ASP:HB2	0.85	0.88
1:A:154:GLY:HA3	2:A:701:FAD:O2P	1.75	0.86
1:A:321:GLY:HA3	1:A:329:THR:H	1.41	0.85
1:B:271:ASP:O	1:B:272:THR:OG1	1.92	0.85
1:B:436:ASP:O	1:B:439:VAL:HG12	1.76	0.85
1:B:439:VAL:HG21	2:B:701:FAD:C7M	2.07	0.85
1:B:373:ASN:HB3	1:B:376:ASP:HB2	1.56	0.84
1:B:375:ASN:O	1:B:377:PRO:HD3	1.77	0.82
1:B:373:ASN:CB	1:B:376:ASP:HB2	2.00	0.82
1:A:321:GLY:HA3	1:A:329:THR:N	1.97	0.80
1:B:143:TYR:H	1:B:195:THR:HG22	1.47	0.80
1:B:154:GLY:HA3	2:B:701:FAD:O2P	1.82	0.80
1:B:561:ILE:HD12	1:B:572:LEU:HB3	1.62	0.80
1:B:372:LEU:HD21	1:B:383:LEU:HD22	1.63	0.79
1:B:206:HIS:NE2	1:B:272:THR:HB	1.97	0.79
1:B:384:GLU:O	1:B:388:THR:HG23	1.83	0.78
1:B:486:GLN:HE21	1:B:488:GLY:H	1.34	0.75
1:B:439:VAL:HG21	2:B:701:FAD:HM73	1.67	0.75
1:B:21:GLN:H	1:B:619:GLN:HE22	1.36	0.74
1:B:206:HIS:NE2	1:B:272:THR:CG2	2.51	0.72
1:B:486:GLN:HE21	1:B:488:GLY:N	1.88	0.72
1:B:377:PRO:HB3	1:B:381:ASN:ND2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:O	1:A:326:THR:HG22	1.89	0.72
1:B:373:ASN:HB3	1:B:376:ASP:CA	2.19	0.72
1:A:156:ASN:H	1:B:319:GLN:HE21	1.38	0.71
1:A:115:PHE:CE2	1:A:119:ILE:HD11	2.26	0.70
1:B:435:ALA:O	1:B:438:VAL:HG22	1.92	0.68
1:B:54:LEU:HD22	1:B:74:ARG:HG2	1.75	0.67
1:A:439:VAL:HG23	2:A:701:FAD:HM83	1.75	0.67
1:B:384:GLU:HG3	1:B:387:VAL:HB	1.77	0.67
1:B:375:ASN:O	1:B:377:PRO:CD	2.43	0.67
1:B:115:PHE:CD1	1:B:198:VAL:HG23	2.30	0.66
1:B:206:HIS:NE2	1:B:272:THR:CB	2.59	0.66
1:B:379:GLN:N	1:B:379:GLN:HE21	1.93	0.66
1:B:138:ALA:HB1	1:B:140:LYS:HE3	1.79	0.65
1:B:374:PRO:CD	1:B:375:ASN:H	2.09	0.65
1:B:486:GLN:NE2	1:B:489:GLN:N	2.45	0.64
1:B:566:ASP:HA	1:B:569:LYS:HD3	1.80	0.64
1:A:321:GLY:CA	1:A:329:THR:H	2.11	0.63
1:B:374:PRO:CG	1:B:375:ASN:H	2.13	0.62
1:A:439:VAL:HG21	2:A:701:FAD:C7M	2.30	0.61
1:A:623:LEU:O	1:A:626:ALA:HB3	2.01	0.61
1:A:179:HIS:HD2	1:A:181:GLY:H	1.48	0.61
1:B:617:ARG:O	1:B:620:VAL:HG23	2.01	0.61
1:A:165:THR:HB	1:A:204:ILE:HB	1.82	0.60
1:A:353:MET:HG3	1:A:557:PHE:HA	1.83	0.60
1:A:115:PHE:CD1	1:A:198:VAL:HG23	2.35	0.60
1:B:54:LEU:CD2	1:B:74:ARG:HG2	2.31	0.60
1:A:115:PHE:CZ	1:A:119:ILE:HD11	2.36	0.60
1:A:557:PHE:O	1:A:561:ILE:HG13	2.03	0.59
1:B:319:GLN:O	1:B:320:PHE:HB2	2.03	0.59
1:B:373:ASN:HB2	1:B:376:ASP:HB3	1.80	0.58
1:B:492:PRO:HG2	1:B:495:GLN:HG3	1.85	0.58
1:B:194:SER:O	1:B:220:ARG:HD2	2.02	0.58
1:B:373:ASN:CG	1:B:376:ASP:HB3	2.15	0.58
1:A:193:THR:HG22	1:A:246:ASP:OD2	2.04	0.58
1:A:439:VAL:CG2	2:A:701:FAD:HM83	2.33	0.58
1:B:379:GLN:HE21	1:B:379:GLN:CA	2.17	0.57
1:B:206:HIS:NE2	1:B:272:THR:HG21	2.17	0.57
1:A:372:LEU:HD21	1:A:382:ASP:CB	2.35	0.57
1:B:72:MET:HE3	1:B:107:ARG:HH11	1.70	0.56
2:B:701:FAD:O4'	2:B:701:FAD:O2'	2.20	0.56
1:A:638:ILE:HA	1:A:645:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:HD21	1:A:382:ASP:HB3	1.88	0.56
1:B:439:VAL:CG2	2:B:701:FAD:HM83	2.33	0.56
1:B:486:GLN:HE22	1:B:489:GLN:N	2.04	0.55
1:B:594:GLU:HB2	1:B:596:ILE:HG12	1.89	0.55
1:B:377:PRO:HB2	1:B:380:LYS:N	2.22	0.55
1:B:378:ALA:O	1:B:379:GLN:HB2	2.05	0.55
1:B:437:TRP:O	1:B:440:GLN:HB2	2.07	0.55
1:B:547:ILE:HD11	1:B:590:ILE:HD13	1.89	0.54
1:B:271:ASP:C	1:B:272:THR:HG1	2.02	0.54
1:B:557:PHE:O	1:B:561:ILE:HG12	2.07	0.54
1:B:561:ILE:CD1	1:B:572:LEU:HB3	2.36	0.54
1:A:72:MET:HG2	1:A:107:ARG:NH2	2.23	0.54
1:B:374:PRO:HD2	1:B:375:ASN:H	1.73	0.54
1:B:72:MET:HE3	1:B:107:ARG:NH1	2.23	0.54
1:A:212:THR:O	1:A:213:ARG:HD3	2.09	0.53
1:B:265:ARG:HB3	1:B:266:TYR:CD1	2.43	0.53
1:B:439:VAL:HG21	2:B:701:FAD:HM71	1.87	0.53
1:A:519:ASP:HA	1:A:522:GLN:OE1	2.09	0.53
1:A:154:GLY:CA	2:A:701:FAD:O2P	2.53	0.52
1:B:190:ALA:HB1	1:B:250:ILE:HD11	1.91	0.52
1:B:569:LYS:N	1:B:570:PRO:HD2	2.24	0.52
1:B:183:THR:HG23	1:B:251:GLN:HG3	1.91	0.52
1:B:374:PRO:HG2	1:B:375:ASN:H	1.74	0.52
1:B:111:HIS:CE1	1:B:139:VAL:HG22	2.45	0.52
1:B:154:GLY:CA	2:B:701:FAD:O2P	2.57	0.52
1:A:413:ASP:OD1	1:B:434:TYR:OH	2.28	0.51
1:A:171:ASP:OD1	1:A:259:ARG:HD3	2.09	0.51
1:B:304:LYS:HD2	1:B:627:PHE:HB3	1.90	0.51
1:B:116:ILE:O	1:B:117:GLY:C	2.46	0.51
1:B:638:ILE:HA	1:B:645:VAL:HG22	1.91	0.51
1:B:374:PRO:CD	1:B:375:ASN:N	2.73	0.51
1:B:374:PRO:CG	1:B:375:ASN:N	2.73	0.50
1:B:377:PRO:HA	1:B:380:LYS:O	2.11	0.50
1:B:206:HIS:CE1	1:B:272:THR:HG21	2.45	0.50
1:B:617:ARG:HD3	1:B:617:ARG:C	2.32	0.50
1:B:385:LYS:O	1:B:389:ASP:OD1	2.29	0.50
1:B:206:HIS:CD2	1:B:272:THR:HB	2.47	0.49
1:B:672:LYS:HB3	1:B:673:PRO:HD3	1.94	0.49
1:B:3:THR:HG22	1:B:327:LYS:NZ	2.27	0.49
1:B:222:VAL:HG23	1:B:223:HIS:CD2	2.48	0.49
1:B:299:SER:HA	1:B:437:TRP:CH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ILE:HD12	1:B:572:LEU:CB	2.40	0.49
1:A:153:HIS:HE1	1:B:328:GLU:OE2	1.95	0.49
1:A:443:TRP:CD1	1:A:443:TRP:C	2.86	0.49
1:B:177:THR:HG23	1:B:182:ALA:HB3	1.95	0.49
1:B:384:GLU:O	1:B:388:THR:N	2.40	0.49
1:A:424:TYR:CZ	1:B:439:VAL:HB	2.49	0.48
1:B:195:THR:HG23	1:B:196:HIS:ND1	2.28	0.48
1:A:316:VAL:HG21	1:A:645:VAL:HG21	1.94	0.48
1:A:638:ILE:HG22	1:A:645:VAL:HG13	1.95	0.48
1:B:642:ASP:HB2	3:B:803:HOH:O	2.14	0.48
1:A:154:GLY:HA3	2:A:701:FAD:P	2.54	0.48
1:A:268:LYS:HB2	1:A:276:THR:HB	1.95	0.47
1:A:275:VAL:O	1:A:275:VAL:CG2	2.62	0.47
1:B:377:PRO:C	1:B:379:GLN:N	2.67	0.47
1:A:168:GLN:NE2	1:A:272:THR:HA	2.29	0.47
2:B:701:FAD:H2'	2:B:701:FAD:H9	1.97	0.47
1:A:362:TRP:CH2	1:A:366:THR:HG21	2.48	0.47
1:B:456:ARG:O	1:B:460:GLN:HG2	2.14	0.47
1:B:464:GLN:NE2	1:B:469:LYS:HE2	2.30	0.47
1:B:206:HIS:CE1	1:B:272:THR:CG2	2.98	0.47
1:B:304:LYS:HB2	1:B:627:PHE:CD2	2.50	0.47
1:B:41:VAL:HB	1:B:96:LEU:HD11	1.95	0.47
1:B:190:ALA:CB	1:B:250:ILE:HD11	2.45	0.47
1:B:617:ARG:O	1:B:620:VAL:CG2	2.62	0.47
1:A:601:ASP:O	1:A:605:ILE:HG12	2.15	0.46
1:B:290:ARG:HA	1:B:293:VAL:HG12	1.98	0.46
1:B:443:TRP:CD1	1:B:443:TRP:C	2.86	0.46
1:A:443:TRP:HD1	1:A:443:TRP:O	1.98	0.46
2:B:701:FAD:H2'	2:B:701:FAD:C9	2.46	0.46
1:B:307:LEU:HD13	1:B:345:LEU:HA	1.98	0.46
1:B:377:PRO:C	1:B:379:GLN:H	2.18	0.45
1:A:496:LEU:HD13	1:A:605:ILE:HD13	1.98	0.45
1:B:383:LEU:CD2	1:B:386:ALA:HB2	2.46	0.45
1:A:71:THR:HG23	1:A:104:THR:HA	1.98	0.45
1:A:439:VAL:HG21	2:A:701:FAD:HM71	1.97	0.45
1:A:205:VAL:HG11	1:A:273:GLY:O	2.16	0.45
1:A:319:GLN:HE22	1:B:153:HIS:HA	1.82	0.45
1:B:306:PHE:CD2	1:B:412:ILE:HD12	2.52	0.45
1:B:506:PHE:CE2	1:B:584:ILE:HD13	2.52	0.45
1:B:529:ASN:HB3	1:B:530:PRO:HD2	1.98	0.45
1:B:205:VAL:O	1:B:205:VAL:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLN:O	1:A:320:PHE:HB2	2.16	0.45
1:A:342:LEU:N	1:A:343:PRO:CD	2.81	0.44
1:B:301:HIS:HA	1:B:304:LYS:HE2	1.98	0.44
1:B:150:GLU:OE2	1:B:162:THR:OG1	2.31	0.44
1:B:443:TRP:HD1	1:B:443:TRP:O	2.01	0.44
1:A:147:ALA:HA	1:A:187:ILE:HD12	1.99	0.44
1:B:372:LEU:HD21	1:B:383:LEU:CD2	2.39	0.44
1:A:439:VAL:HG21	2:A:701:FAD:HM73	1.98	0.44
1:B:339:ARG:CZ	1:B:609:VAL:HG23	2.48	0.44
1:A:115:PHE:CE1	1:A:198:VAL:HG23	2.52	0.44
1:B:301:HIS:O	1:B:304:LYS:HG2	2.17	0.44
1:A:168:GLN:HE21	1:A:272:THR:HA	1.82	0.44
1:B:524:LEU:HD12	1:B:537:LEU:HD11	1.99	0.44
1:B:154:GLY:HA3	2:B:701:FAD:H5'2	1.99	0.43
1:B:339:ARG:NH1	1:B:609:VAL:HG23	2.32	0.43
1:A:471:VAL:HG12	1:A:472:GLY:N	2.32	0.43
1:A:496:LEU:HD13	1:A:605:ILE:CD1	2.49	0.43
1:B:492:PRO:HG2	1:B:495:GLN:CG	2.48	0.43
1:A:588:THR:HG22	1:B:589:GLY:HA3	2.01	0.43
1:B:408:CYS:HB3	1:B:437:TRP:CE2	2.53	0.43
1:A:346:ALA:HB1	1:A:579:PHE:HB2	2.01	0.43
1:A:672:LYS:HB3	1:A:673:PRO:HD3	2.01	0.43
1:B:142:PHE:HA	1:B:195:THR:HG21	2.01	0.42
1:B:120:ARG:HB2	1:B:128:PHE:CE1	2.54	0.42
1:A:473:ALA:HA	1:A:476:GLN:HG3	2.01	0.42
1:B:373:ASN:ND2	1:B:376:ASP:OD1	2.49	0.42
1:B:595:ASN:CG	1:B:595:ASN:O	2.58	0.42
1:B:8:ASP:N	1:B:9:PRO:CD	2.83	0.42
1:B:288:LEU:HD23	1:B:394:PHE:HZ	1.84	0.42
1:A:326:THR:HG23	1:A:326:THR:O	2.20	0.42
1:A:438:VAL:HG13	1:B:416:ARG:NH1	2.35	0.42
1:B:340:ARG:O	1:B:344:LEU:HD22	2.19	0.42
2:B:701:FAD:H9	2:B:701:FAD:C2'	2.49	0.42
1:B:486:GLN:NE2	1:B:489:GLN:H	2.14	0.42
1:A:149:THR:OG1	2:A:701:FAD:H1'1	2.20	0.41
1:A:319:GLN:HE22	1:B:154:GLY:H	1.68	0.41
1:A:372:LEU:HD21	1:A:382:ASP:HB2	2.00	0.41
1:A:543:GLN:O	1:A:547:ILE:HG12	2.20	0.41
1:A:179:HIS:CD2	1:A:181:GLY:H	2.33	0.41
1:B:192:HIS:O	1:B:225:HIS:HE1	2.03	0.41
1:B:186:TRP:HB3	2:B:701:FAD:C9A	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASN:HB2	1:B:263:LEU:HD12	2.02	0.41
1:A:638:ILE:HG22	1:A:645:VAL:CG1	2.51	0.41
1:B:373:ASN:HB3	1:B:376:ASP:O	2.20	0.41
1:A:424:TYR:HE1	1:B:438:VAL:HG23	1.86	0.41
1:B:147:ALA:HA	1:B:187:ILE:HD12	2.01	0.41
1:B:289:ILE:HG21	1:B:362:TRP:CZ2	2.55	0.41
1:B:71:THR:HG23	1:B:104:THR:HA	2.03	0.41
1:A:192:HIS:O	1:A:225:HIS:HE1	2.03	0.41
1:A:275:VAL:O	1:A:275:VAL:HG23	2.21	0.41
1:A:319:GLN:NE2	1:B:154:GLY:H	2.17	0.41
1:B:210:TYR:CZ	1:B:274:VAL:HG21	2.55	0.41
1:A:179:HIS:HD2	1:A:181:GLY:N	2.16	0.41
1:B:383:LEU:HD23	1:B:386:ALA:CB	2.51	0.41
1:B:204:ILE:HA	1:B:208:LYS:O	2.21	0.41
1:B:375:ASN:HD22	1:B:375:ASN:HA	1.65	0.40
1:A:362:TRP:CZ2	1:A:366:THR:HG21	2.56	0.40
1:A:321:GLY:N	1:A:329:THR:H	2.20	0.40
1:B:375:ASN:C	1:B:377:PRO:HD3	2.40	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	685/709 (97%)	670 (98%)	15 (2%)	0	100	100
1	B	678/709 (96%)	654 (96%)	23 (3%)	1 (0%)	51	73
All	All	1363/1418 (96%)	1324 (97%)	38 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	376	ASP

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	584/603 (97%)	534 (91%)	50 (9%)	10 20
1	B	580/603 (96%)	514 (89%)	66 (11%)	5 11
All	All	1164/1206 (96%)	1048 (90%)	116 (10%)	7 15

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	46	SER
1	A	57	THR
1	A	87	GLU
1	A	90	SER
1	A	105	ARG
1	A	112	ASN
1	A	120	ARG
1	A	133	LYS
1	A	157	LEU
1	A	165	THR
1	A	193	THR
1	A	197	CYS
1	A	199	CYS
1	A	208	LYS
1	A	213	ARG
1	A	225	HIS
1	A	233	ILE
1	A	261	ASN
1	A	275	VAL
1	A	282	GLN
1	A	284	THR
1	A	322	THR

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Mol	Chain	Res	Type
1	A	325	ASP
1	A	326	THR
1	A	347	TYR
1	A	365	THR
1	A	369	ILE
1	A	383	LEU
1	A	385	LYS
1	A	438	VAL
1	A	443	TRP
1	A	474	SER
1	A	475	ILE
1	A	481	LYS
1	A	484	ILE
1	A	527	THR
1	A	528	LEU
1	A	537	LEU
1	A	550	ARG
1	A	557	PHE
1	A	567	ASP
1	A	593	ARG
1	A	604	LEU
1	A	617	ARG
1	A	620	VAL
1	A	652	LYS
1	A	655	GLN
1	A	682	ASP
1	A	687	LEU
1	B	2	THR
1	B	3	THR
1	B	36	GLU
1	B	46	SER
1	B	72	MET
1	B	90	SER
1	B	105	ARG
1	B	110	ILE
1	B	112	ASN
1	B	133	LYS
1	B	137	VAL
1	B	140	LYS
1	B	169	ASP
1	B	193	THR
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	213	ARG
1	B	225	HIS
1	B	238	LYS
1	B	250	ILE
1	B	260	GLN
1	B	265	ARG
1	B	276	THR
1	B	356	ASP
1	B	370	LEU
1	B	372	LEU
1	B	375	ASN
1	B	376	ASP
1	B	379	GLN
1	B	383	LEU
1	B	384	GLU
1	B	391	LYS
1	B	410	LYS
1	B	443	TRP
1	B	444	GLU
1	B	474	SER
1	B	475	ILE
1	B	489	GLN
1	B	491	THR
1	B	506	PHE
1	B	513	ASN
1	B	523	GLU
1	B	535	GLU
1	B	543	GLN
1	B	550	ARG
1	B	551	GLN
1	B	557	PHE
1	B	563	THR
1	B	565	LYS
1	B	566	ASP
1	B	573	LEU
1	B	574	LYS
1	B	603	ASP
1	B	606	ASN
1	B	617	ARG
1	B	620	VAL
1	B	635	ASN
1	B	640	SER

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Mol	Chain	Res	Type
1	B	642	ASP
1	B	644	ASN
1	B	645	VAL
1	B	647	GLU
1	B	652	LYS
1	B	681	ASP
1	B	682	ASP
1	B	687	LEU
1	B	688	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	168	GLN
1	A	179	HIS
1	A	221	ASN
1	A	225	HIS
1	A	247	ASN
1	A	261	ASN
1	A	301	HIS
1	A	319	GLN
1	A	486	GLN
1	A	635	ASN
1	A	654	ASN
1	A	656	GLN
1	B	21	GLN
1	B	127	GLN
1	B	176	ASN
1	B	179	HIS
1	B	223	HIS
1	B	225	HIS
1	B	247	ASN
1	B	319	GLN
1	B	373	ASN
1	B	375	ASN
1	B	379	GLN
1	B	381	ASN
1	B	428	ASN
1	B	464	GLN
1	B	486	GLN
1	B	512	ASN

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Mol	Chain	Res	Type
1	B	551	GLN
1	B	606	ASN
1	B	619	GLN
1	B	635	ASN
1	B	644	ASN
1	B	654	ASN
1	B	655	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 monosaccharides in this entry.

5.6 Ligand geometry

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	701	-	53,58,58	1.41	5 (9%)	68,89,89	1.34	12 (17%)
2	FAD	A	701	-	53,58,58	1.45	6 (11%)	68,89,89	1.26	9 (13%)

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	701	-	-	10/30/50/50	0/6/6/6
2	FAD	A	701	-	-	6/30/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C9A-C5X	4.06	1.48	1.41
2	B	701	FAD	C4-N3	-3.84	1.31	1.38
2	A	701	FAD	C9A-C5X	3.82	1.47	1.41
2	A	701	FAD	C4-N3	-3.57	1.32	1.38
2	A	701	FAD	C5X-N5	-3.46	1.32	1.39
2	B	701	FAD	C5X-N5	-3.00	1.33	1.39
2	A	701	FAD	C8-C7	2.97	1.48	1.40
2	B	701	FAD	C2-N3	-2.92	1.32	1.39
2	B	701	FAD	C8-C7	2.79	1.47	1.40
2	A	701	FAD	C2-N3	-2.66	1.32	1.39
2	A	701	FAD	C6-C7	-2.24	1.36	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	FAD	N3A-C2A-N1A	-3.33	123.47	128.68
2	B	701	FAD	C4A-C5A-N7A	-3.13	106.13	109.40
2	B	701	FAD	C4X-C10-N1	-2.97	117.84	124.73
2	A	701	FAD	C4A-C5A-N7A	-2.95	106.33	109.40
2	A	701	FAD	N3A-C2A-N1A	-2.85	124.23	128.68
2	B	701	FAD	C4-C4X-N5	2.75	122.15	118.23
2	A	701	FAD	C4X-C10-N1	-2.71	118.44	124.73
2	B	701	FAD	C10-N1-C2	2.56	122.03	116.90
2	A	701	FAD	O4-C4-C4X	-2.49	120.01	126.60
2	B	701	FAD	C3B-C2B-C1B	2.48	104.71	100.98
2	B	701	FAD	C4X-C4-N3	2.45	119.41	113.19
2	B	701	FAD	C4X-C10-N10	2.37	119.95	116.48
2	A	701	FAD	C10-N1-C2	2.28	121.46	116.90
2	B	701	FAD	C4-N3-C2	-2.26	121.46	125.64
2	A	701	FAD	C4-C4X-N5	2.15	121.30	118.23
2	A	701	FAD	C9A-N10-C10	-2.13	117.45	120.77
2	B	701	FAD	O4-C4-C4X	-2.09	121.06	126.60
2	B	701	FAD	O2-C2-N1	-2.08	118.38	121.83
2	A	701	FAD	C4X-C10-N10	2.07	119.50	116.48
2	A	701	FAD	C4X-C4-N3	2.04	118.37	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	FAD	C9A-N10-C10	-2.01	117.64	120.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C1'-C2'-C3'-O3'
2	A	701	FAD	C1'-C2'-C3'-C4'
2	B	701	FAD	C1'-C2'-C3'-O3'
2	B	701	FAD	C1'-C2'-C3'-C4'
2	B	701	FAD	C5'-O5'-P-O1P
2	B	701	FAD	C5'-O5'-P-O2P
2	A	701	FAD	O2'-C2'-C3'-O3'
2	A	701	FAD	O2'-C2'-C3'-C4'
2	B	701	FAD	O2'-C2'-C3'-C4'
2	B	701	FAD	O2'-C2'-C3'-O3'
2	B	701	FAD	C5'-O5'-P-O3P
2	A	701	FAD	PA-O3P-P-O2P
2	B	701	FAD	PA-O3P-P-O2P
2	A	701	FAD	PA-O3P-P-O1P
2	B	701	FAD	PA-O3P-P-O1P
2	B	701	FAD	C2'-C1'-N10-C10

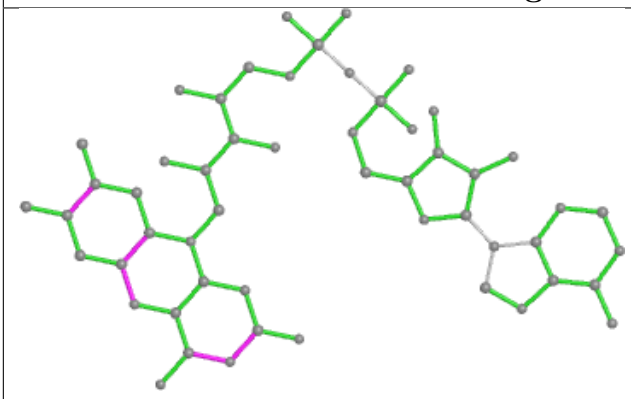
There are no ring outliers.

2 monomers are involved in 22 short contacts:

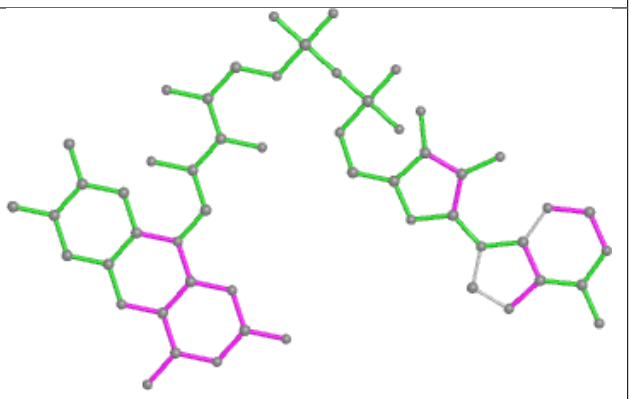
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FAD	13	0
2	A	701	FAD	9	0

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 then 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.

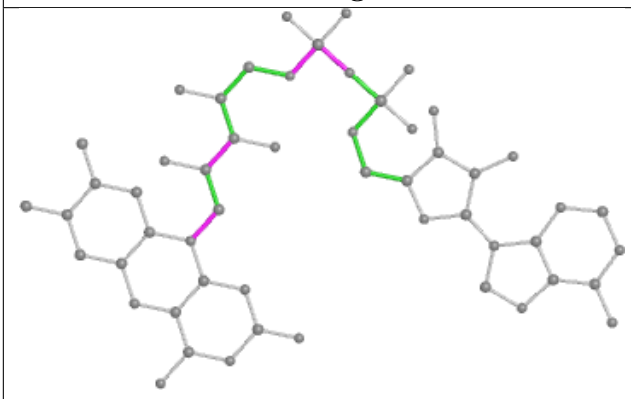
Ligand FAD B 701



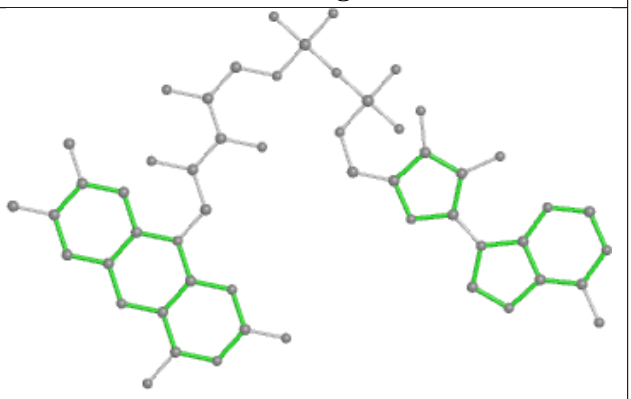
Bond lengths



Bond angles

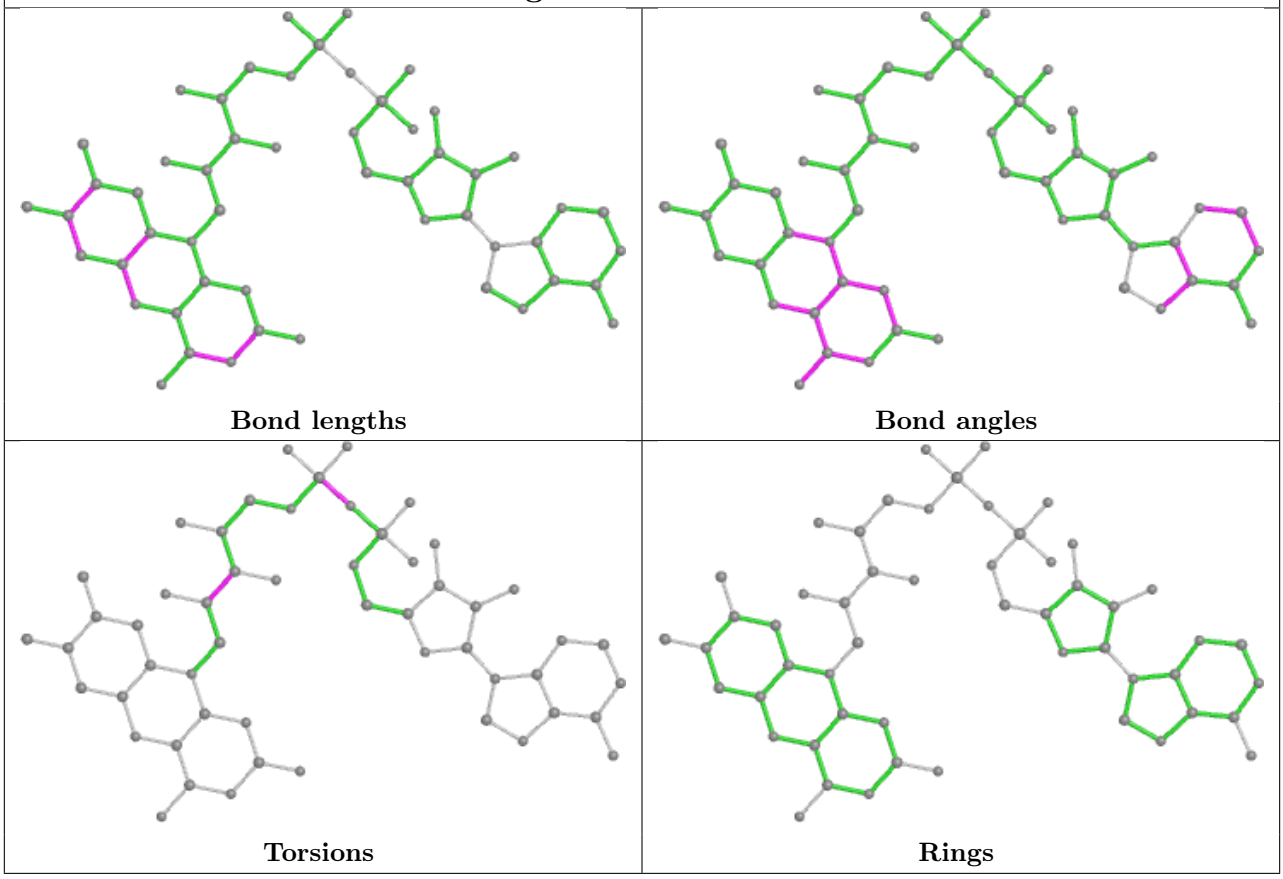


Torsions



Rings

Ligand FAD A 701



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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	687/709 (96%)	-0.36	9 (1%) 77 79	20, 35, 78, 112	0
1	B	682/709 (96%)	-0.16	20 (2%) 51 55	22, 42, 82, 114	0
All	All	1369/1418 (96%)	-0.26	29 (2%) 63 66	20, 38, 81, 114	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	ASP	7.7
1	B	278	PRO	6.6
1	B	272	THR	3.9
1	B	371	ALA	3.9
1	A	276	THR	3.8
1	A	682	ASP	3.7
1	B	285	TYR	3.6
1	B	373	ASN	3.6
1	B	368	ARG	3.5
1	B	271	ASP	3.4
1	B	374	PRO	3.2
1	B	370	LEU	3.1
1	B	379	GLN	3.0
1	A	489	GLN	3.0
1	B	378	ALA	2.9
1	A	688	ASP	2.8
1	A	685	CYS	2.7
1	A	281	ASP	2.6
1	B	277	LYS	2.5
1	B	382	ASP	2.5
1	B	287	ALA	2.5
1	A	377	PRO	2.4
1	B	601	ASP	2.4
1	B	362	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	364	GLU	2.3
1	B	384	GLU	2.2
1	A	2	THR	2.2
1	B	681	ASP	2.2
1	B	435	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

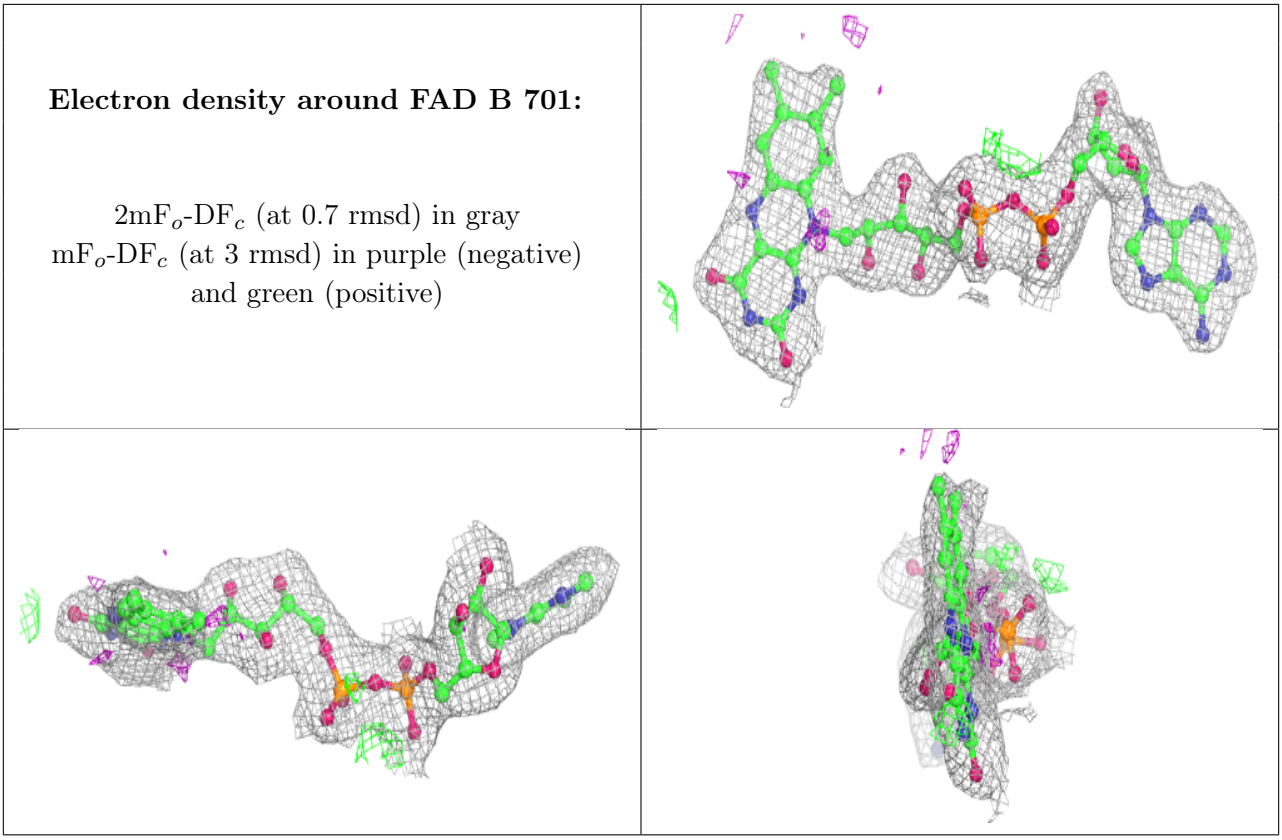
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	B	701	53/53	0.96	0.11	26,33,39,40	0
2	FAD	A	701	53/53	0.97	0.13	19,26,32,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

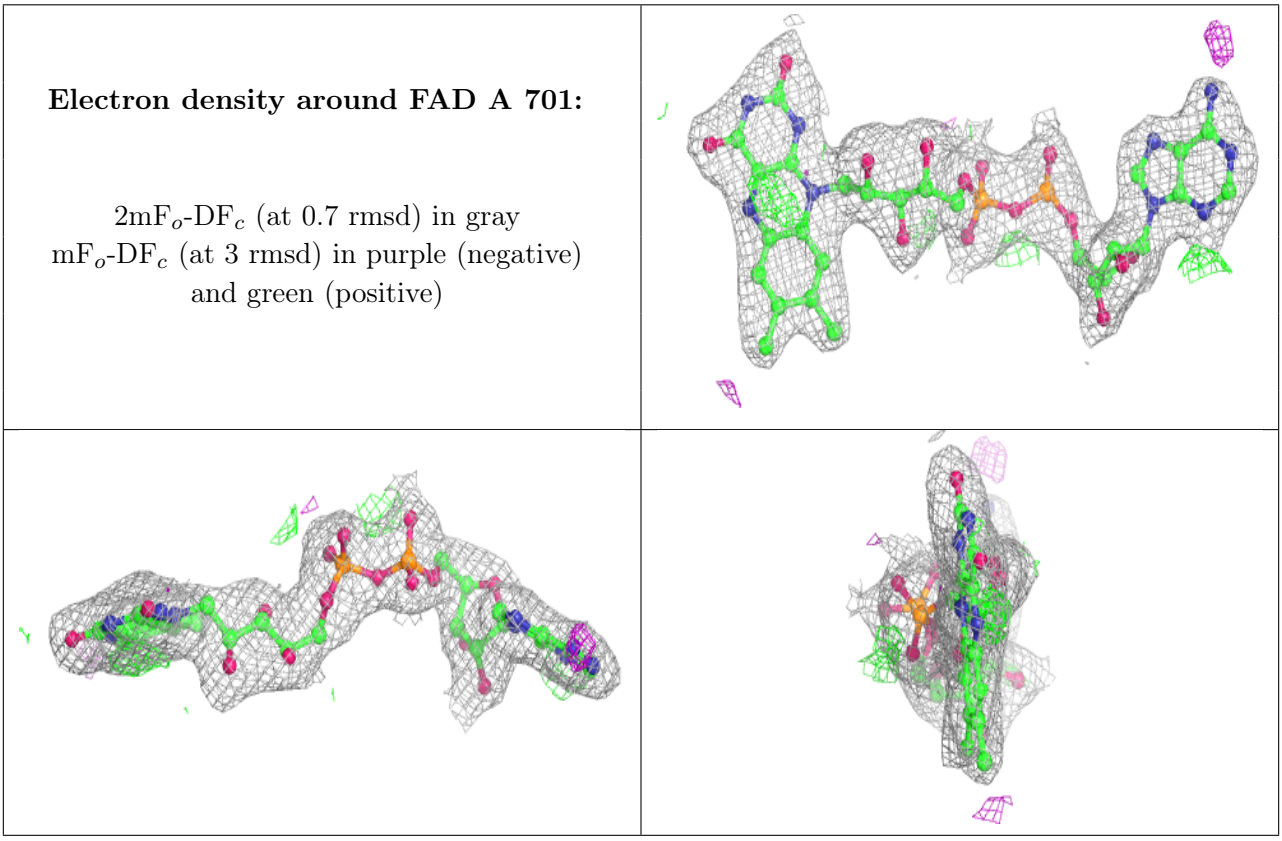
Electron density around FAD B 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.