Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 08:35 PM EST

PDB ID	:	3OC4
Title	:	Crystal Structure of a pyridine nucleotide-disulfide family oxidoreductase from the Enterococcus faecalis V583
Authors	:	Kumaran, D.; Baumann, K.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-08-09
Resolution	:	2.60 Å(reported)

The following versions of software and data (see references ⓘ) 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	:	2.16
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)	:	2.16
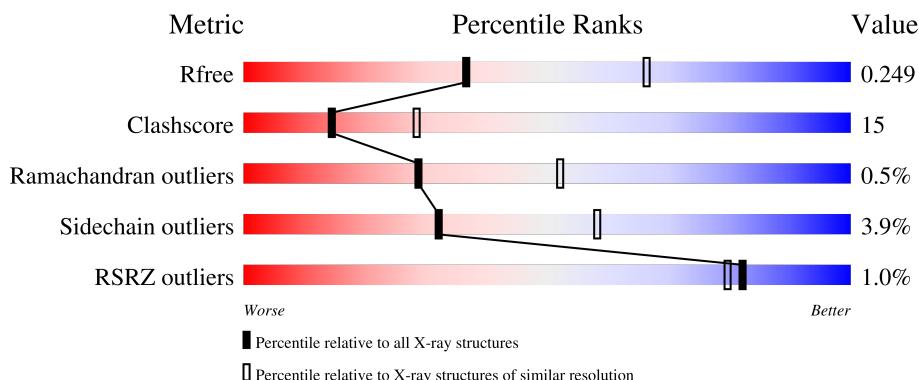
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
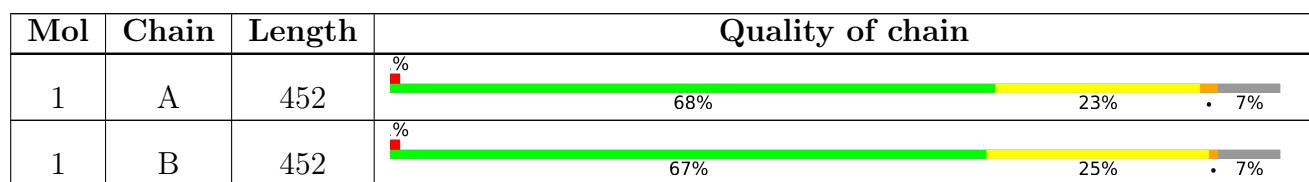
The reported resolution of this entry is 2.60 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.249
Clashscore		15
Ramachandran outliers		0.5%
Sidechain outliers		3.9%
RSRZ outliers		1.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	452	% 68% 23% • 7%
1	B	452	% 67% 25% • 7%

2 Entity composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6914 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.
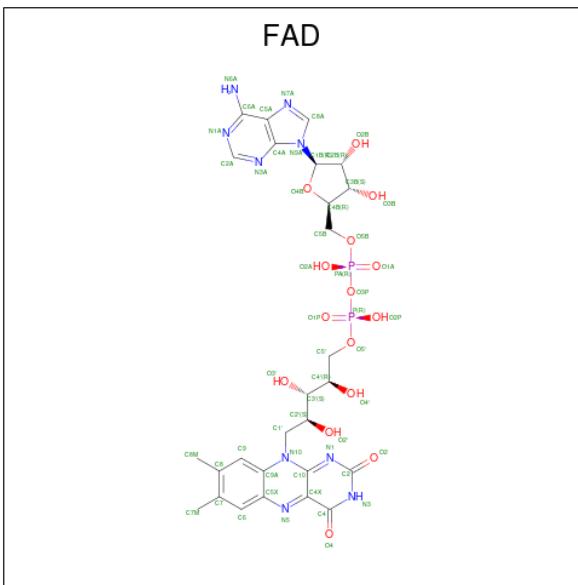
- Molecule 1 is a protein called Oxidoreductase, pyridine nucleotide-disulfide family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	Se	0	0	0
			3316	2120	549	636	4	7			
1	B	421	Total	C	N	O	S	Se	0	0	0
			3305	2111	547	636	4	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MSE	-	expression tag	UNP Q833L5
A	-2	SER	-	expression tag	UNP Q833L5
A	-1	LEU	-	expression tag	UNP Q833L5
A	444	GLY	-	expression tag	UNP Q833L5
A	445	HIS	-	expression tag	UNP Q833L5
A	446	HIS	-	expression tag	UNP Q833L5
A	447	HIS	-	expression tag	UNP Q833L5
A	448	HIS	-	expression tag	UNP Q833L5
A	449	HIS	-	expression tag	UNP Q833L5
A	450	HIS	-	expression tag	UNP Q833L5
B	-3	MSE	-	expression tag	UNP Q833L5
B	-2	SER	-	expression tag	UNP Q833L5
B	-1	LEU	-	expression tag	UNP Q833L5
B	444	GLY	-	expression tag	UNP Q833L5
B	445	HIS	-	expression tag	UNP Q833L5
B	446	HIS	-	expression tag	UNP Q833L5
B	447	HIS	-	expression tag	UNP Q833L5
B	448	HIS	-	expression tag	UNP Q833L5
B	449	HIS	-	expression tag	UNP Q833L5
B	450	HIS	-	expression tag	UNP Q833L5

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

FAD

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 SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
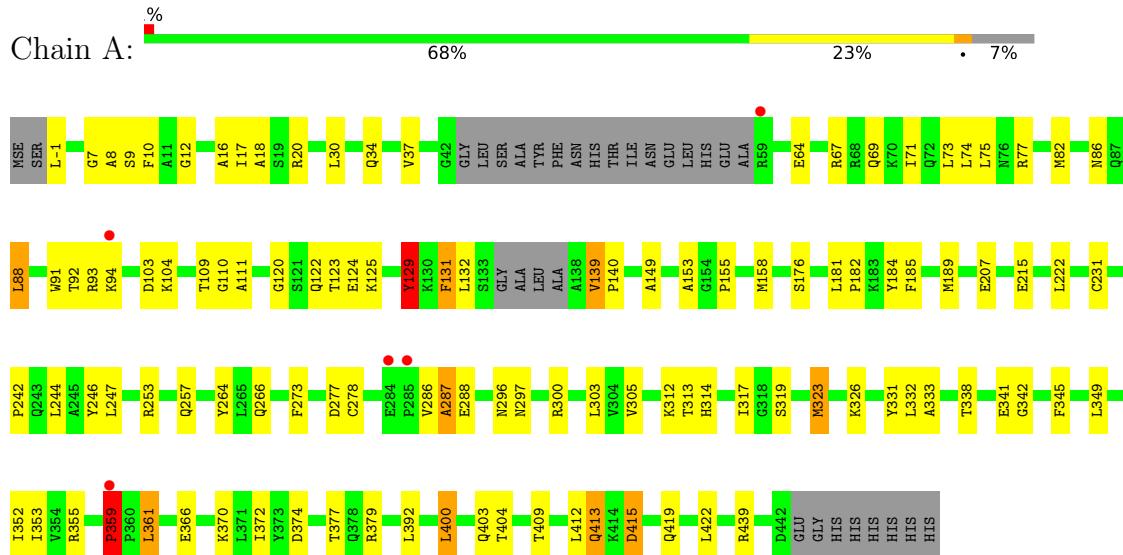
• Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total	O	0	0
			90	90		
4	B	95	Total	O	0	0
			95	95		
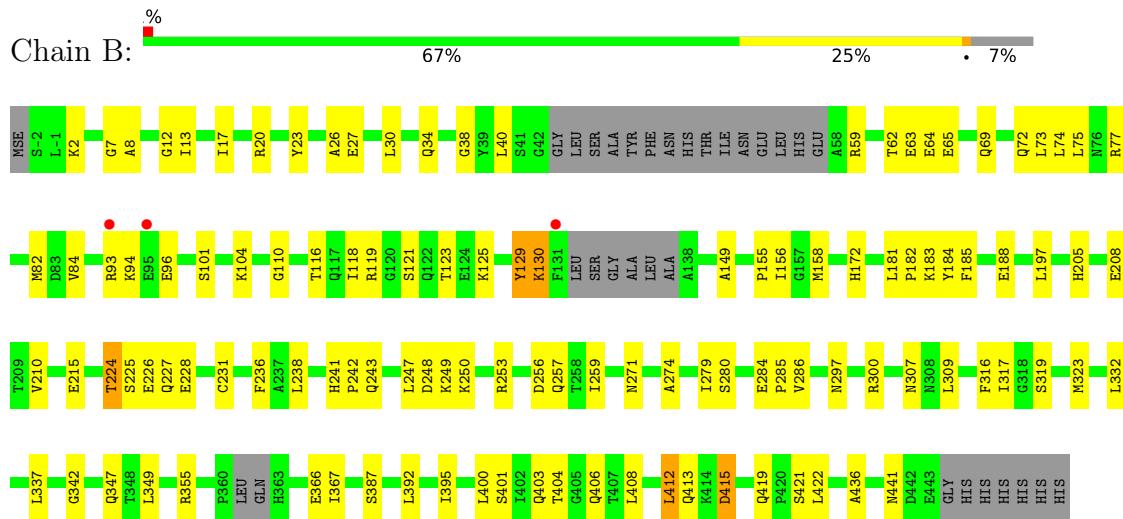
3 Residue-property plots ⓘ

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 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: Oxidoreductase, pyridine nucleotide-disulfide family

Chain A:

- Molecule 1: Oxidoreductase, pyridine nucleotide-disulfide family

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	213.69Å 213.69Å 149.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.13 – 2.60 44.13 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.13-2.60) 97.5 (44.13-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.94 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.251 0.220 , 0.249	Depositor DCC
R_{free} test set	2589 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6914	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 12.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NA, 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	0.41	1/3362 (0.0%)	0.68	1/4543 (0.0%)
1	B	0.38	0/3350	0.64	0/4525
All	All	0.39	1/6712 (0.0%)	0.66	1/9068 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	CYS	CB-SG	-6.06	1.72	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	LEU	CA-CB-CG	5.12	127.07	115.30

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	3316	0	3373	121	0
1	B	3305	0	3353	98	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	90	0	0	3	0
4	B	95	0	0	5	0
All	All	6914	0	6788	208	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 15.

All (208) 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:224:THR:HG22	1:B:227:GLN:H	1.16	1.04
1:B:224:THR:HG23	1:B:226:GLU:H	1.19	1.03
1:A:123:THR:HG22	1:A:125:LYS:H	1.24	1.02
1:A:419:GLN:HG2	1:A:422:LEU:HD12	1.45	0.95
1:A:415:ASP:H	1:B:403:GLN:HE22	1.11	0.95
1:B:123:THR:HG22	1:B:125:LYS:H	1.32	0.93
1:A:374:ASP:HB3	1:A:377:THR:HG22	1.48	0.93
1:A:153:ALA:HB1	1:A:158:MSE:HE3	1.55	0.87
1:A:403:GLN:HE22	1:B:415:ASP:H	1.24	0.83
1:B:224:THR:HG22	1:B:227:GLN:N	1.96	0.81
1:A:153:ALA:HB1	1:A:158:MSE:CE	2.11	0.79
1:A:64:GLU:HA	1:A:67:ARG:HH11	1.46	0.78
1:A:129:TYR:O	1:A:132:LEU:HB2	1.84	0.77
1:B:224:THR:CG2	1:B:226:GLU:H	1.95	0.76
1:A:120:GLY:HA2	1:A:122:GLN:HE22	1.51	0.74
1:A:286:VAL:O	1:A:286:VAL:HG12	1.87	0.73
1:B:419:GLN:HG2	1:B:422:LEU:HD12	1.72	0.72
1:A:129:TYR:CD2	1:A:132:LEU:HD22	2.25	0.72
1:B:419:GLN:NE2	1:B:421:SER:H	1.88	0.71
1:A:64:GLU:HG3	1:A:67:ARG:HH12	1.57	0.70
1:A:439:ARG:HG2	1:A:439:ARG:HH11	1.56	0.70
1:A:286:VAL:O	1:A:288:GLU:HG2	1.92	0.69
1:B:419:GLN:HE21	1:B:421:SER:H	1.39	0.69
1:A:110:GLY:HA2	1:A:277:ASP:HB2	1.76	0.67
1:A:317:ILE:H	1:B:413:GLN:NE2	1.93	0.67
1:A:244:LEU:HB2	1:A:253:ARG:HH22	1.59	0.67
1:A:244:LEU:HB2	1:A:253:ARG:NH2	2.10	0.67
1:A:288:GLU:HG3	1:A:345:PHE:CE2	2.30	0.66
1:A:374:ASP:CB	1:A:377:THR:HG22	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:MSE:HE1	1:A:246:TYR:HE1	1.61	0.66
1:A:34:GLN:O	1:A:75:LEU:HB3	1.96	0.65
1:A:317:ILE:H	1:B:413:GLN:HE22	1.42	0.65
1:A:189:MSE:HE3	1:A:353:ILE:CD1	2.27	0.65
1:B:59:ARG:HH22	1:B:63:GLU:HG3	1.62	0.65
1:B:38:GLY:O	1:B:59:ARG:HA	1.96	0.65
1:B:93:ARG:NH1	1:B:94:LYS:HE3	2.13	0.64
1:A:419:GLN:HG2	1:A:422:LEU:CD1	2.26	0.63
1:A:439:ARG:HG2	1:A:439:ARG:NH1	2.13	0.63
1:A:342:GLY:HA3	1:A:349:LEU:HD12	1.80	0.63
1:B:172:HIS:ND1	1:B:205:HIS:HE1	1.97	0.62
1:B:274:ALA:HB3	1:B:279:ILE:HD11	1.81	0.62
1:B:118:ILE:HD12	1:B:210:VAL:O	1.99	0.62
1:B:208:GLU:OE1	1:B:224:THR:HG21	1.99	0.62
1:A:415:ASP:H	1:B:403:GLN:NE2	1.91	0.61
1:B:342:GLY:HA3	1:B:349:LEU:HD12	1.81	0.61
1:A:123:THR:HG23	1:A:215:GLU:OE1	2.01	0.61
1:B:183:LYS:HE2	1:B:183:LYS:HA	1.82	0.61
1:A:131:PHE:N	1:A:131:PHE:CD2	2.66	0.61
1:A:8:ALA:HB3	1:A:37:VAL:HG11	1.82	0.60
1:B:82:MSE:HG3	1:B:248:ASP:HB2	1.83	0.60
1:A:139:VAL:HG23	1:A:140:PRO:HD2	1.84	0.60
1:A:155:PRO:HG3	1:A:323:MSE:HE2	1.82	0.60
1:B:116:THR:OG1	1:B:118:ILE:HG12	2.00	0.60
1:B:184:TYR:CG	1:B:323:MSE:HE3	2.37	0.60
1:A:253:ARG:HD2	4:A:479:HOH:O	2.01	0.59
1:A:153:ALA:HA	1:A:158:MSE:HE2	1.85	0.59
1:A:17:ILE:HG23	1:A:69:GLN:HE22	1.68	0.59
1:B:224:THR:HG23	1:B:226:GLU:N	2.04	0.59
1:A:153:ALA:CB	1:A:158:MSE:CE	2.80	0.58
1:B:248:ASP:OD1	1:B:250:LYS:HB2	2.03	0.58
1:A:413:GLN:HE22	1:B:316:PHE:HA	1.68	0.58
1:B:184:TYR:CD2	1:B:323:MSE:HE3	2.38	0.58
1:A:297:ASN:OD1	1:A:319:SER:HB2	2.04	0.58
1:A:352:ILE:HD12	1:A:439:ARG:HD3	1.86	0.58
1:B:74:LEU:HB3	1:B:77:ARG:HD2	1.86	0.57
1:A:189:MSE:CE	1:A:353:ILE:HD13	2.33	0.57
1:A:92:THR:HG23	4:A:499:HOH:O	2.04	0.56
1:A:75:LEU:N	1:A:75:LEU:HD12	2.20	0.56
1:A:338:THR:OG1	1:A:341:GLU:HG2	2.06	0.56
1:B:401:SER:O	1:B:404:THR:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:HD2	2:B:500:FAD:HM82	1.87	0.56
1:A:73:LEU:HB3	1:A:75:LEU:HD11	1.88	0.56
1:B:17:ILE:HD12	1:B:69:GLN:HE22	1.70	0.56
1:A:111:ALA:HA	1:A:242:PRO:HA	1.88	0.55
1:A:377:THR:HG23	1:A:379:ARG:H	1.69	0.55
1:B:59:ARG:HE	1:B:62:THR:HG22	1.71	0.55
1:A:123:THR:HG22	1:A:125:LYS:N	2.08	0.55
1:A:16:ALA:HB1	1:A:71:ILE:HD13	1.88	0.55
1:B:404:THR:CG2	1:B:406:GLN:HG3	2.36	0.55
1:A:131:PHE:HD2	1:A:131:PHE:N	2.04	0.54
1:B:256:ASP:O	1:B:257:GLN:HB2	2.08	0.54
1:A:359:PRO:O	1:A:361:LEU:N	2.41	0.54
1:A:244:LEU:HD12	1:A:253:ARG:NH2	2.22	0.54
1:A:184:TYR:CD1	1:A:323:MSE:HG2	2.43	0.54
1:A:355:ARG:HD3	1:A:366:GLU:OE2	2.07	0.54
1:B:82:MSE:HE2	1:B:84:VAL:CG2	2.37	0.53
1:B:224:THR:CG2	1:B:227:GLN:H	2.05	0.53
1:B:247:LEU:HD23	1:B:253:ARG:HD2	1.90	0.53
1:B:355:ARG:HG2	1:B:366:GLU:OE2	2.08	0.53
1:A:266:GLN:HG3	1:A:273:PHE:CE1	2.44	0.53
1:A:153:ALA:CB	1:A:158:MSE:HE3	2.34	0.53
1:B:280:SER:HB2	4:B:480:HOH:O	2.08	0.53
1:A:415:ASP:N	1:B:403:GLN:HE22	1.93	0.53
1:B:156:ILE:HG13	4:B:461:HOH:O	2.09	0.52
1:B:20:ARG:NH2	1:B:26:ALA:H	2.06	0.52
1:A:7:GLY:O	1:A:12:GLY:HA3	2.09	0.52
1:A:64:GLU:HG3	1:A:67:ARG:NH1	2.23	0.51
1:A:120:GLY:HA2	1:A:122:GLN:NE2	2.22	0.51
1:B:73:LEU:HD22	1:B:75:LEU:HD21	1.92	0.51
1:A:189:MSE:HE3	1:A:353:ILE:HD13	1.92	0.51
1:A:93:ARG:HG2	1:A:93:ARG:HH11	1.76	0.51
1:B:419:GLN:HE21	1:B:421:SER:N	2.08	0.51
1:B:236:PHE:CE2	1:B:238:LEU:HB2	2.45	0.51
1:B:307:ASN:HB3	4:B:505:HOH:O	2.09	0.51
1:B:236:PHE:CZ	1:B:238:LEU:HB2	2.45	0.51
1:B:185:PHE:CZ	1:B:332:LEU:HB3	2.46	0.51
1:B:412:LEU:C	1:B:412:LEU:HD23	2.31	0.51
1:B:20:ARG:HD2	1:B:69:GLN:O	2.11	0.50
1:A:313:THR:HG22	1:A:314:HIS:CD2	2.46	0.50
1:B:123:THR:HG23	1:B:215:GLU:CD	2.32	0.50
1:A:18:ALA:HB2	1:A:303:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ILE:HD12	4:B:487:HOH:O	2.11	0.50
1:B:110:GLY:O	1:B:242:PRO:HA	2.12	0.49
1:A:439:ARG:CG	1:A:439:ARG:HH11	2.24	0.49
1:A:82:MSE:HE1	1:A:246:TYR:CE1	2.44	0.49
1:B:20:ARG:CD	1:B:69:GLN:O	2.61	0.49
1:A:82:MSE:HE3	1:A:246:TYR:CD1	2.47	0.48
1:A:413:GLN:NE2	1:B:317:ILE:H	2.11	0.48
1:B:130:LYS:HD2	2:B:500:FAD:C8M	2.43	0.48
1:A:86:ASN:O	1:A:88:LEU:HD13	2.13	0.48
1:A:185:PHE:CZ	1:A:332:LEU:HB3	2.49	0.48
1:B:129:TYR:O	1:B:130:LYS:CB	2.62	0.48
1:B:13:ILE:O	1:B:17:ILE:HG12	2.13	0.48
1:B:82:MSE:HE2	1:B:84:VAL:HG22	1.94	0.48
1:A:122:GLN:H	1:A:122:GLN:CD	2.18	0.47
1:B:75:LEU:O	1:B:77:ARG:NH1	2.47	0.47
1:A:92:THR:O	1:A:92:THR:HG23	2.14	0.47
1:B:118:ILE:HB	1:B:121:SER:HB3	1.96	0.47
1:B:94:LYS:O	1:B:96:GLU:HG3	2.15	0.47
1:A:370:LYS:HE2	1:A:372:ILE:HD11	1.95	0.47
1:A:8:ALA:HB2	1:A:30:LEU:HG	1.96	0.47
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.80	0.47
1:A:333:ALA:HB2	1:A:392:LEU:HD22	1.97	0.47
1:B:123:THR:HG22	1:B:125:LYS:N	2.15	0.46
1:A:264:TYR:CG	1:A:312:LYS:HG3	2.50	0.46
1:B:2:LYS:HE3	1:B:101:SER:O	2.16	0.46
1:A:74:LEU:HB3	1:A:77:ARG:HD2	1.97	0.46
1:A:286:VAL:O	1:A:286:VAL:CG1	2.58	0.46
1:A:82:MSE:HE3	1:A:246:TYR:HD1	1.79	0.46
1:B:155:PRO:HD2	4:B:461:HOH:O	2.14	0.46
1:B:158:MSE:HE1	1:B:197:LEU:HD11	1.98	0.46
1:B:279:ILE:CG2	1:B:280:SER:N	2.79	0.46
1:B:34:GLN:NE2	1:B:34:GLN:HA	2.31	0.46
1:A:404:THR:HG21	1:B:404:THR:HG21	1.98	0.45
1:A:153:ALA:CA	1:A:158:MSE:CE	2.95	0.45
1:A:370:LYS:HE2	1:A:372:ILE:CD1	2.47	0.45
1:A:20:ARG:HD2	1:A:69:GLN:O	2.16	0.45
1:A:93:ARG:HH11	1:A:94:LYS:HG3	1.80	0.45
1:A:326:LYS:HD2	1:A:331:TYR:CE1	2.52	0.45
1:B:104:LYS:NZ	1:B:271:ASN:ND2	2.65	0.45
1:A:222:LEU:H	1:A:222:LEU:HD12	1.81	0.45
1:B:392:LEU:O	1:B:395:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:HG3	1:A:345:PHE:HE2	1.80	0.45
1:B:149:ALA:HB2	1:B:231:CYS:SG	2.57	0.44
1:A:82:MSE:CE	1:A:246:TYR:CE1	3.00	0.44
1:A:264:TYR:CD1	1:A:312:LYS:HG3	2.52	0.44
1:A:93:ARG:HG2	1:A:94:LYS:HG3	1.99	0.44
1:A:123:THR:CG2	1:A:125:LYS:HB2	2.47	0.44
1:A:244:LEU:HD12	1:A:253:ARG:HH21	1.83	0.44
1:A:412:LEU:C	1:A:412:LEU:HD23	2.37	0.44
1:B:104:LYS:HG2	1:B:309:LEU:HB3	1.99	0.44
1:A:184:TYR:CE1	1:A:323:MSE:HG2	2.52	0.44
1:B:27:GLU:HG2	1:B:72:GLN:HE22	1.83	0.44
1:A:286:VAL:O	1:A:288:GLU:CG	2.63	0.44
1:A:93:ARG:CG	1:A:93:ARG:HH11	2.31	0.43
1:A:377:THR:HG23	1:A:379:ARG:N	2.31	0.43
1:A:77:ARG:HD3	1:A:91:TRP:CE2	2.52	0.43
1:A:277:ASP:OD2	2:A:500:FAD:H5'1	2.18	0.43
1:A:75:LEU:O	1:A:77:ARG:HG3	2.18	0.43
1:A:64:GLU:HA	1:A:67:ARG:NH1	2.24	0.43
1:A:9:SER:OG	1:A:10:PHE:N	2.49	0.43
1:B:408:LEU:HD22	1:B:436:ALA:HB3	2.00	0.43
1:A:149:ALA:HB2	1:A:231:CYS:SG	2.58	0.43
1:A:75:LEU:HD12	1:A:75:LEU:H	1.82	0.43
1:A:286:VAL:CG1	1:A:345:PHE:CD2	3.02	0.42
2:A:500:FAD:H3'	4:A:459:HOH:O	2.19	0.42
1:B:181:LEU:HD22	1:B:323:MSE:CE	2.50	0.42
1:A:413:GLN:O	1:B:300:ARG:HD2	2.20	0.42
1:A:71:ILE:O	1:A:73:LEU:HD12	2.19	0.42
1:B:23:TYR:HB3	1:B:26:ALA:HB2	2.00	0.42
1:A:413:GLN:HE22	1:B:317:ILE:H	1.68	0.42
1:B:297:ASN:OD1	1:B:319:SER:HB2	2.19	0.42
1:A:296:ASN:HD22	1:A:300:ARG:HH11	1.68	0.41
1:B:8:ALA:HB2	1:B:30:LEU:HG	2.01	0.41
1:A:400:LEU:HB3	1:B:400:LEU:HD23	2.01	0.41
1:B:181:LEU:N	1:B:182:PRO:CD	2.82	0.41
1:B:27:GLU:CG	1:B:72:GLN:HE22	2.33	0.41
1:A:181:LEU:N	1:A:182:PRO:CD	2.82	0.41
1:B:241:HIS:HB3	1:B:242:PRO:HD2	2.01	0.41
1:B:413:GLN:HE21	1:B:413:GLN:HB2	1.75	0.41
1:A:377:THR:CG2	1:A:379:ARG:H	2.34	0.41
1:B:7:GLY:O	1:B:12:GLY:HA3	2.21	0.41
1:A:103:ASP:O	1:A:104:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:THR:HG23	1:B:225:SER:N	2.34	0.41
1:B:284:GLU:HB2	1:B:285:PRO:HD3	2.02	0.41
1:A:129:TYR:CE2	1:A:132:LEU:HD22	2.56	0.41
1:A:286:VAL:HG11	1:A:345:PHE:CD2	2.56	0.41
1:A:244:LEU:HD13	1:A:247:LEU:HD22	2.03	0.41
1:B:104:LYS:HE3	1:B:309:LEU:O	2.20	0.41
1:A:153:ALA:O	1:A:158:MSE:HE3	2.21	0.40
1:A:176:SER:O	1:A:207:GLU:HA	2.21	0.40
1:B:367:ILE:HA	1:B:387:SER:HB2	2.04	0.40
1:B:400:LEU:O	1:B:404:THR:HB	2.20	0.40
1:A:286:VAL:O	1:A:287:ALA:C	2.60	0.40
1:A:181:LEU:HD22	1:A:323:MSE:CE	2.51	0.40
1:B:286:VAL:HG11	1:B:337:LEU:HD11	2.03	0.40
1:B:93:ARG:HH11	1:B:93:ARG:HG2	1.86	0.40
1:B:259:ILE:O	1:B:279:ILE:HD13	2.21	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	416/452 (92%)	387 (93%)	26 (6%)	3 (1%)	22	43
1	B	413/452 (91%)	396 (96%)	16 (4%)	1 (0%)	47	71
All	All	829/904 (92%)	783 (94%)	42 (5%)	4 (0%)	29	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ALA
1	A	359	PRO
1	B	130	LYS

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Mol	Chain	Res	Type
1	A	129	TYR

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	364/379 (96%)	349 (96%)	15 (4%)	30	56
1	B	362/379 (96%)	349 (96%)	13 (4%)	35	61
All	All	726/758 (96%)	698 (96%)	28 (4%)	32	58

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	LEU
1	A	109	THR
1	A	124	GLU
1	A	129	TYR
1	A	131	PHE
1	A	139	VAL
1	A	257	GLN
1	A	305	VAL
1	A	323	MSE
1	A	359	PRO
1	A	361	LEU
1	A	400	LEU
1	A	409	THR
1	A	413	GLN
1	A	415	ASP
1	B	40	LEU
1	B	64	GLU
1	B	65	GLU
1	B	129	TYR
1	B	188	GLU
1	B	224	THR
1	B	228	GLU

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Mol	Chain	Res	Type
1	B	243	GLN
1	B	249	LYS
1	B	347	GLN
1	B	412	LEU
1	B	415	ASP
1	B	441	ASN

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	69	GLN
1	A	72	GLN
1	A	86	ASN
1	A	98	GLN
1	A	122	GLN
1	A	194	GLN
1	A	239	ASN
1	A	254	ASN
1	A	271	ASN
1	A	296	ASN
1	A	378	GLN
1	A	403	GLN
1	A	406	GLN
1	A	413	GLN
1	A	430	ASN
1	B	34	GLN
1	B	69	GLN
1	B	72	GLN
1	B	87	GLN
1	B	117	GLN
1	B	205	HIS
1	B	239	ASN
1	B	252	GLN
1	B	254	ASN
1	B	271	ASN
1	B	347	GLN
1	B	378	GLN
1	B	403	GLN
1	B	406	GLN
1	B	413	GLN
1	B	419	GLN
1	B	430	ASN

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Mol	Chain	Res	Type
1	B	441	ASN

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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	500	-	51,58,58	1.84	11 (21%)	60,89,89	1.87	9 (15%)
2	FAD	A	500	-	51,58,58	1.72	9 (17%)	60,89,89	1.89	9 (15%)

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	500	-	-	1/30/50/50	0/6/6/6
2	FAD	A	500	-	-	1/30/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C9A-N10	6.15	1.46	1.38
2	A	500	FAD	C9A-N10	5.60	1.46	1.38
2	B	500	FAD	C10-N1	4.77	1.39	1.33
2	B	500	FAD	C4X-C10	4.57	1.43	1.38
2	A	500	FAD	C4X-C10	4.33	1.43	1.38
2	A	500	FAD	C10-N1	4.19	1.38	1.33
2	B	500	FAD	C4X-N5	3.74	1.38	1.33
2	A	500	FAD	C4-N3	3.68	1.39	1.33
2	A	500	FAD	C4X-N5	3.57	1.38	1.33
2	B	500	FAD	C4-N3	3.25	1.38	1.33
2	B	500	FAD	C1'-N10	2.94	1.51	1.48
2	A	500	FAD	O4B-C1B	2.63	1.44	1.41
2	B	500	FAD	C4A-N3A	2.62	1.39	1.35
2	A	500	FAD	C6-C7	2.60	1.44	1.37
2	B	500	FAD	C2A-N3A	2.51	1.36	1.32
2	A	500	FAD	C4A-N3A	2.46	1.39	1.35
2	B	500	FAD	C6-C7	2.34	1.43	1.37
2	A	500	FAD	C2A-N3A	2.29	1.35	1.32
2	B	500	FAD	O4B-C1B	2.27	1.44	1.41
2	B	500	FAD	C9-C8	2.12	1.43	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	C4-N3-C2	7.01	121.06	115.14
2	A	500	FAD	C4-N3-C2	6.72	120.81	115.14
2	B	500	FAD	C4X-N5-C5X	6.27	123.04	116.77
2	A	500	FAD	C4X-N5-C5X	6.18	122.95	116.77
2	B	500	FAD	N3A-C2A-N1A	-5.18	120.58	128.68
2	A	500	FAD	N3A-C2A-N1A	-5.08	120.74	128.68
2	A	500	FAD	C1'-N10-C9A	5.01	122.24	118.29
2	B	500	FAD	C1'-N10-C9A	4.76	122.04	118.29
2	A	500	FAD	C4-C4X-C10	-3.77	117.46	119.95
2	B	500	FAD	C4-C4X-C10	-3.63	117.55	119.95
2	A	500	FAD	C4-C4X-N5	3.07	122.11	118.60
2	B	500	FAD	C4-C4X-N5	2.96	121.98	118.60
2	A	500	FAD	C4X-C4-N3	-2.67	119.78	123.43
2	B	500	FAD	C9A-N10-C10	-2.46	118.68	121.91
2	B	500	FAD	C4X-C4-N3	-2.37	120.19	123.43
2	A	500	FAD	C9A-N10-C10	-2.32	118.87	121.91
2	A	500	FAD	C4A-C5A-N7A	-2.27	107.04	109.40
2	B	500	FAD	C4A-C5A-N7A	-2.04	107.27	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:
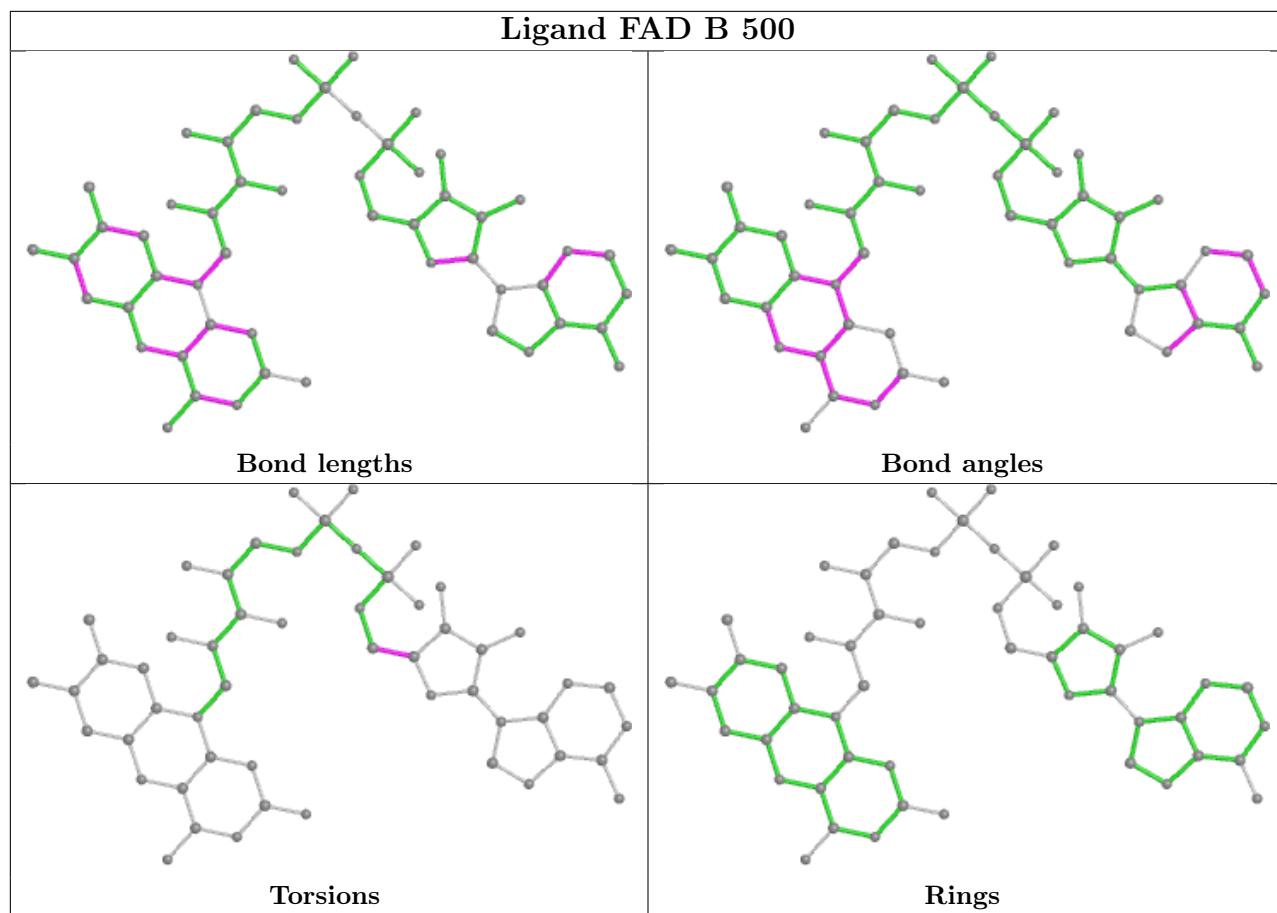
Mol	Chain	Res	Type	Atoms
2	A	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	O4B-C4B-C5B-O5B
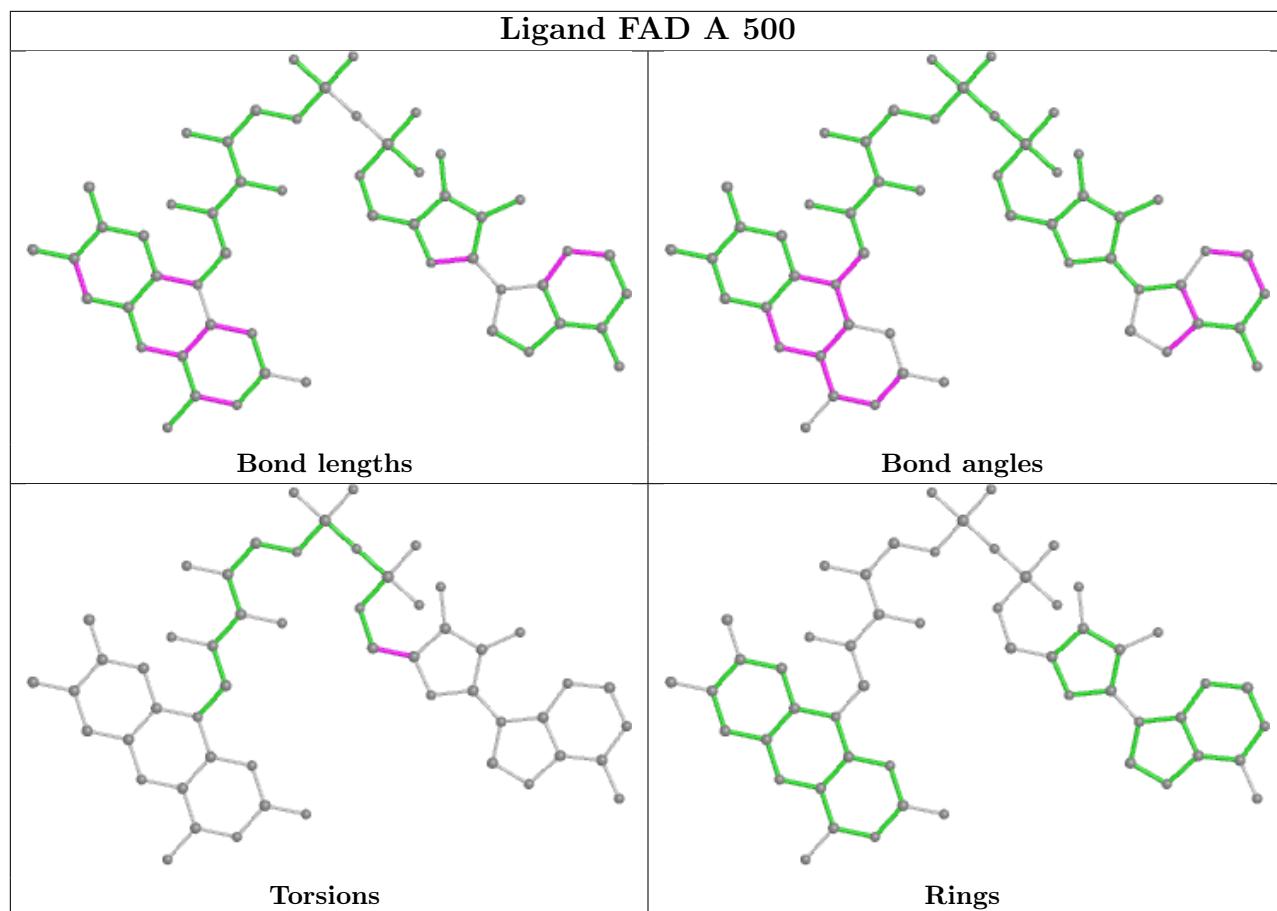
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	FAD	2	0
2	A	500	FAD	2	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 500

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 500

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	415/452 (91%)	-0.21	5 (1%)	79	76	18, 38, 78, 97	0
1	B	414/452 (91%)	-0.28	3 (0%)	87	86	20, 39, 72, 89	0
All	All	829/904 (91%)	-0.24	8 (0%)	82	80	18, 39, 74, 97	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	PHE	2.9
1	A	285	PRO	2.8
1	A	59	ARG	2.7
1	A	359	PRO	2.6
1	B	95	GLU	2.6
1	B	93	ARG	2.5
1	A	94	LYS	2.4
1	A	284	GLU	2.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.
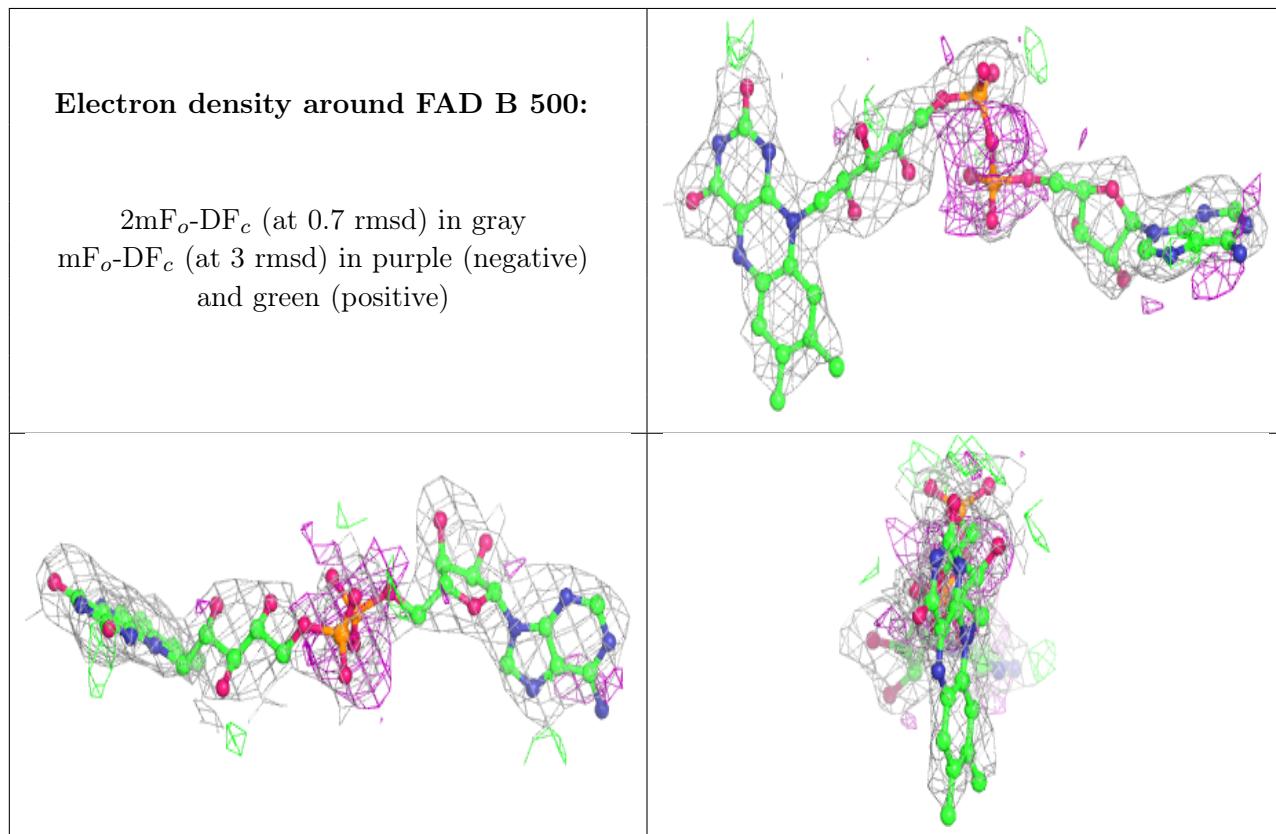
## 6.4 Ligands ⓘ
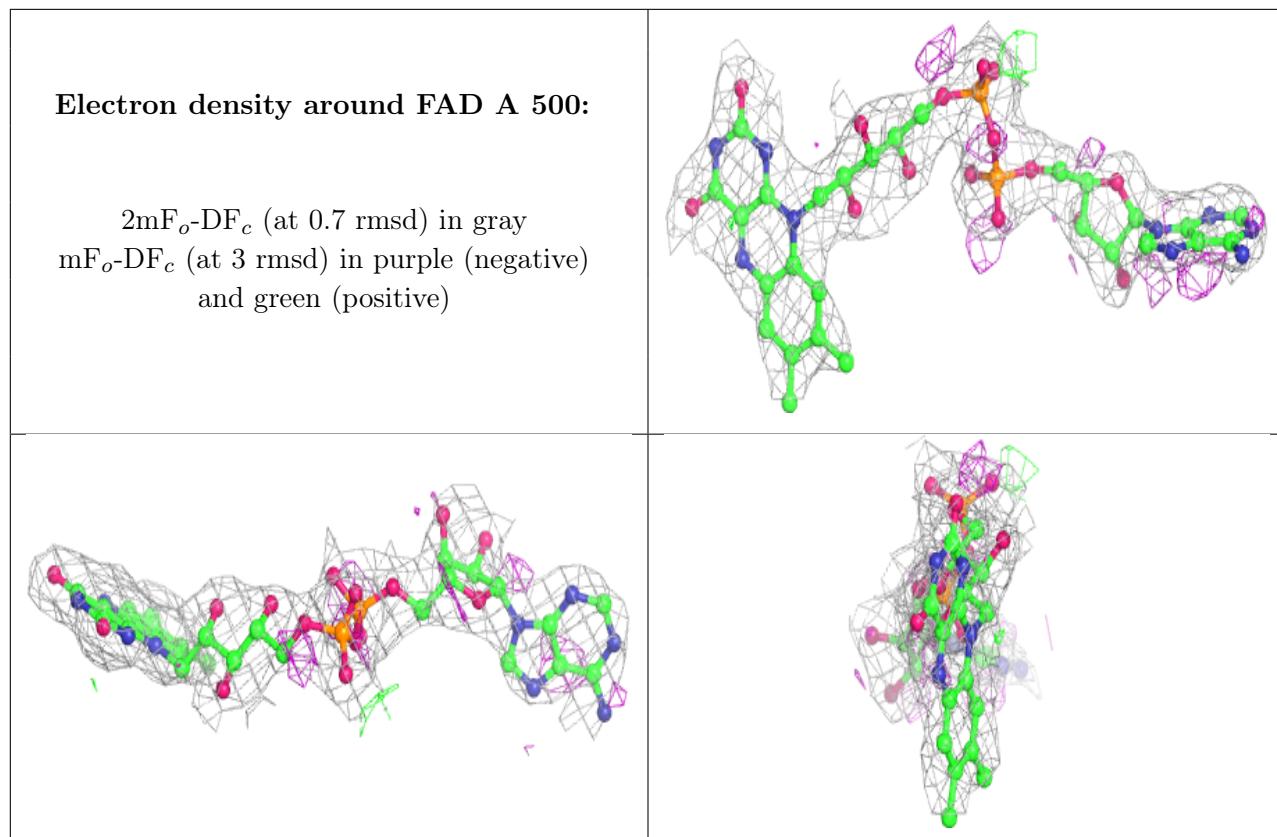
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th 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	500	53/53	0.86	0.21	56,64,68,69	0
3	NA	B	501	1/1	0.88	0.12	45,45,45,45	0
3	NA	A	501	1/1	0.91	0.07	35,35,35,35	0
2	FAD	A	500	53/53	0.92	0.16	46,50,57,57	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 500:

$2mF_o$-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 500:

$2mF_o$-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.