Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2024 – 03:38 pm GMT

PDB ID	:	8R2U
Title	:	Crystal structure of hydroquinone-2-hydroxylase from Trametes versicolor (TvMNX3)
Authors	:	Zahn, M.; Kuatsjah, E.; Salvachua, D.
Deposited on	:	2023-11-07
Resolution	:	2.41 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:

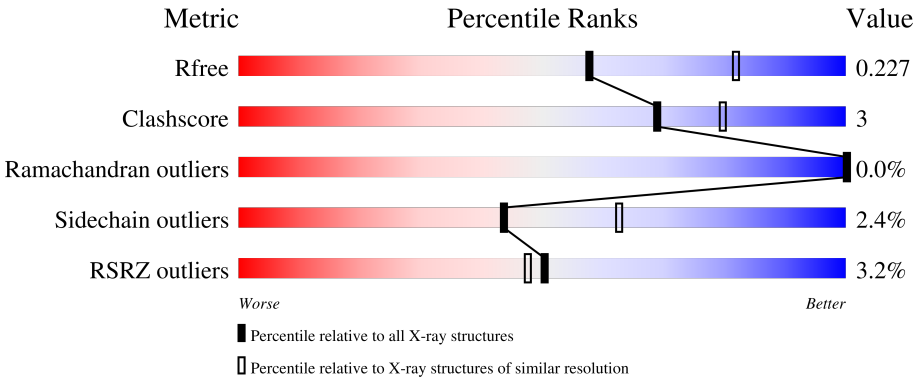
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.41 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}	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	624	4% 89% 7%
1	B	624	3% 90% 6%
1	C	624	3% 89% 7%
1	D	624	3% 88% 7%

2 Entry composition

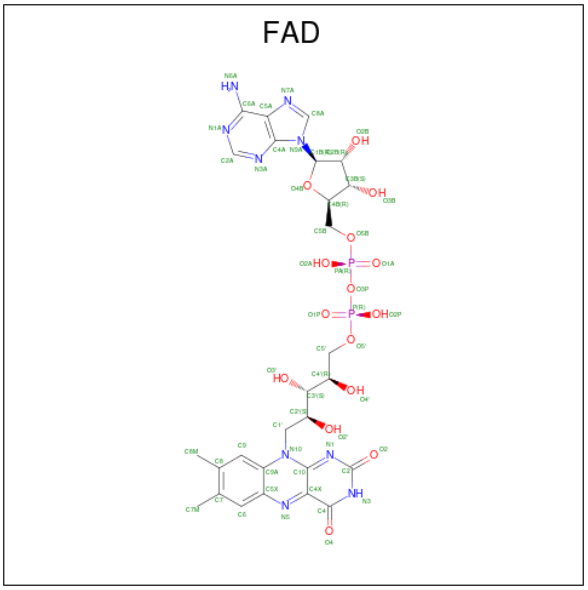
There are 3 unique types of molecules in this entry. The entry contains 19323 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phenol 2-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	1	0
			4674	2963	820	874	17			
1	B	602	Total	C	N	O	S	0	1	0
			4674	2963	820	874	17			
1	C	602	Total	C	N	O	S	0	0	0
			4668	2959	820	872	17			
1	D	602	Total	C	N	O	S	0	1	0
			4674	2963	820	874	17			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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		

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

- Molecule 3 is water.

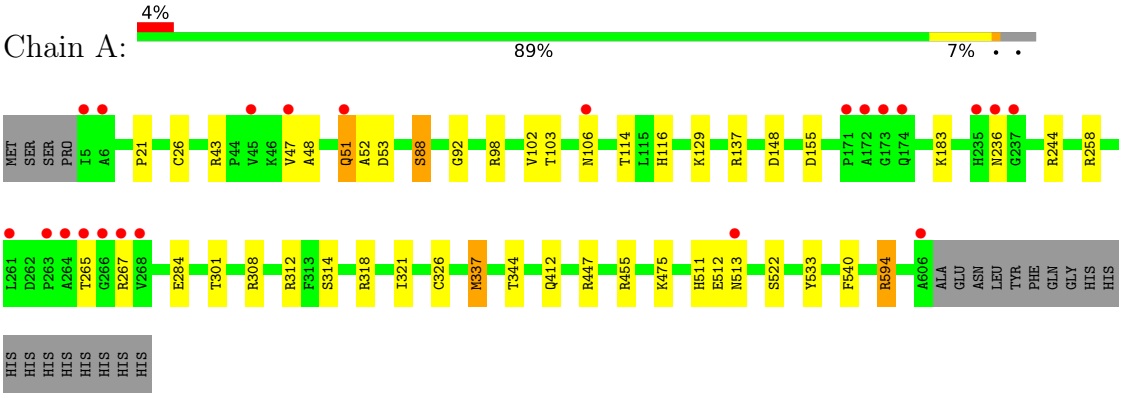
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	105	Total	O	0	0
			105	105		
3	C	97	Total	O	0	0
			97	97		
3	D	99	Total	O	0	0
			99	99		

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.

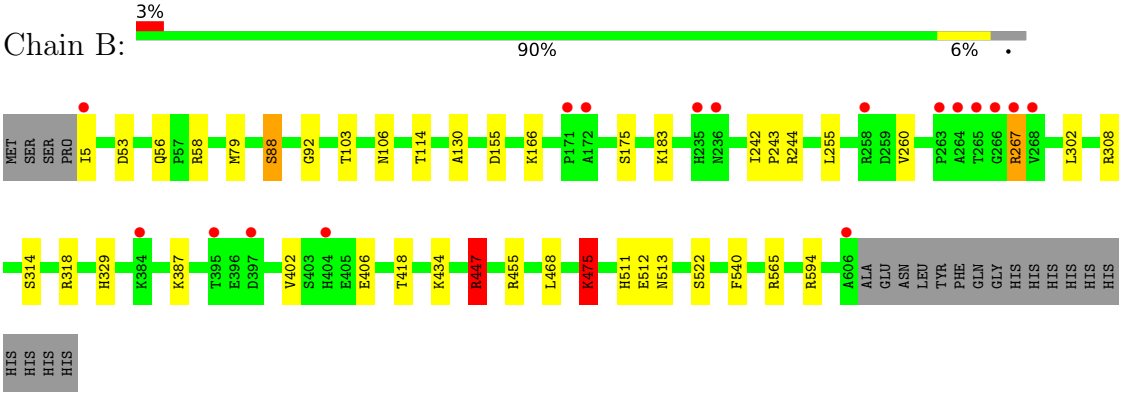
• Molecule 1: Phenol 2-monooxygenase

Chain A:



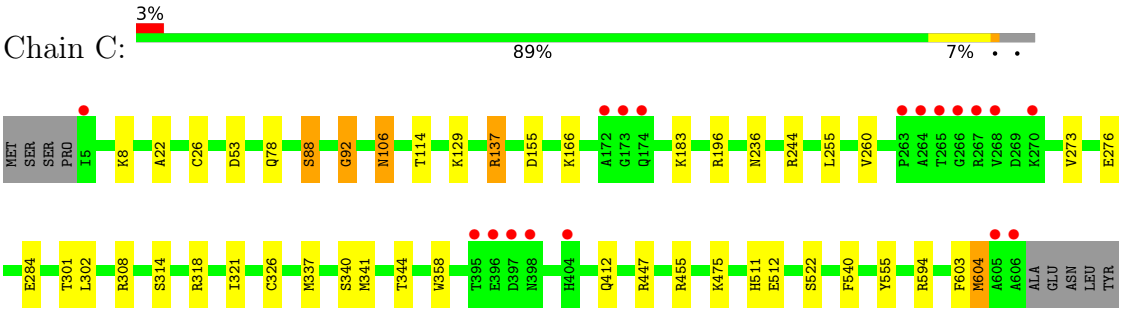
• Molecule 1: Phenol 2-monooxygenase

Chain B:

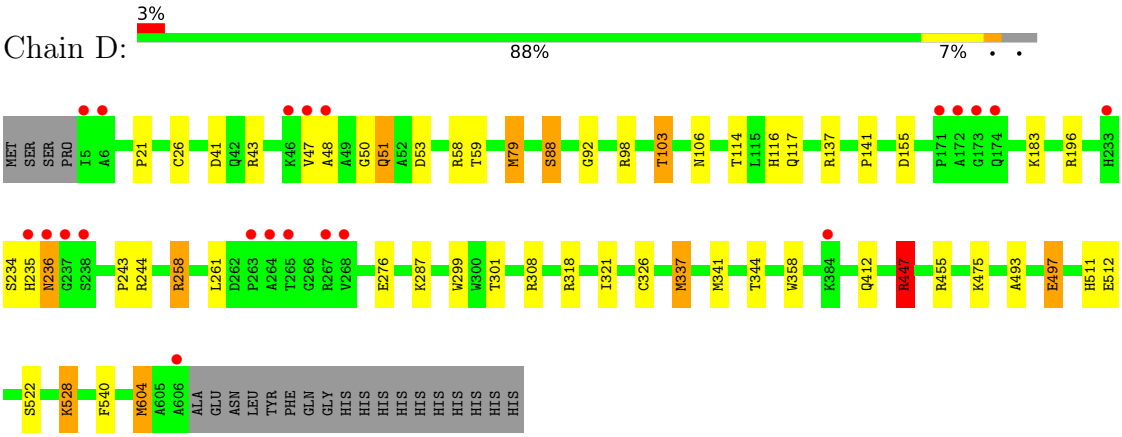


• Molecule 1: Phenol 2-monooxygenase

Chain C:



• Molecule 1: Phenol 2-monooxygenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.17Å 178.19Å 124.72Å 90.00° 129.30° 90.00°	Depositor
Resolution (Å)	107.88 – 2.41 107.88 – 2.41	Depositor EDS
% Data completeness (in resolution range)	68.7 (107.88-2.41) 68.7 (107.88-2.41)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.192 , 0.226 0.196 , 0.227	Depositor DCC
R_{free} test set	3986 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.3	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	0.92	EDS
Total number of atoms	19323	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.47	0/4790	0.77	5/6504 (0.1%)
1	B	0.47	0/4790	0.75	2/6504 (0.0%)
1	C	0.47	0/4781	0.76	2/6492 (0.0%)
1	D	0.49	0/4790	0.77	4/6504 (0.1%)
All	All	0.48	0/19151	0.76	13/26004 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	6
1	C	0	6
1	D	0	5
All	All	0	22

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	GLN	CB-CA-C	-9.56	91.28	110.40
1	A	106	ASN	CB-CA-C	-7.16	96.07	110.40
1	D	106	ASN	CB-CA-C	-6.78	96.84	110.40
1	C	106	ASN	CB-CA-C	-6.61	97.17	110.40
1	C	196	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	98	ARG	CB-CG-CD	-5.49	97.32	111.60
1	D	98	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	475	LYS	CD-CE-NZ	-5.31	99.49	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	ASP	CB-CA-C	-5.29	99.82	110.40
1	D	196	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	51	GLN	N-CA-CB	5.25	120.06	110.60
1	B	166	LYS	CB-CG-CD	5.20	125.13	111.60
1	D	497	GLU	CB-CA-C	-5.12	100.15	110.40

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	244	ARG	Sidechain
1	A	308	ARG	Sidechain
1	A	455	ARG	Sidechain
1	A	594	ARG	Sidechain
1	B	244	ARG	Sidechain
1	B	267	ARG	Sidechain
1	B	308	ARG	Sidechain
1	B	447	ARG	Sidechain
1	B	455	ARG	Sidechain
1	B	565	ARG	Sidechain
1	C	137	ARG	Sidechain
1	C	244	ARG	Sidechain
1	C	308	ARG	Sidechain
1	C	455	ARG	Sidechain
1	C	594	ARG	Sidechain
1	C	92	GLY	Peptide
1	D	244	ARG	Sidechain
1	D	258	ARG	Sidechain
1	D	308	ARG	Sidechain
1	D	447	ARG	Sidechain
1	D	455	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4674	0	4584	32	0
1	B	4674	0	4584	26	0
1	C	4668	0	4578	24	0
1	D	4674	0	4584	43	0
2	A	53	0	31	12	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	11	0
3	A	120	0	0	2	0
3	B	105	0	0	3	0
3	C	97	0	0	4	0
3	D	99	0	0	6	0
All	All	19323	0	18454	127	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 3.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLN:HB2	2:A:701:FAD:N1	1.62	1.15
1:A:51:GLN:HB2	2:A:701:FAD:C10	1.84	1.06
1:D:235:HIS:CE1	1:D:236:ASN:HB3	2.10	0.86
1:D:51:GLN:HB2	1:D:117:GLN:OE1	1.75	0.85
1:D:51:GLN:HA	2:D:701:FAD:C4X	2.08	0.84
1:A:43:ARG:HH11	1:A:47:VAL:HG13	1.43	0.83
1:A:51:GLN:CB	2:A:701:FAD:N1	2.43	0.82
1:D:43:ARG:HH11	1:D:47:VAL:HG13	1.44	0.81
1:A:51:GLN:HB3	2:A:701:FAD:H2'	1.66	0.75
1:C:166:LYS:HE3	3:C:842:HOH:O	1.87	0.74
1:B:79:MET:HE1	1:B:243:PRO:HD2	1.69	0.73
1:D:103:THR:OG1	3:D:801:HOH:O	2.07	0.71
1:D:528:LYS:HE2	3:D:804:HOH:O	1.89	0.71
1:A:265:THR:OG1	1:A:267:ARG:NH1	2.24	0.70
1:B:56:GLN:HG3	3:B:899:HOH:O	1.92	0.70
1:D:301:THR:HG21	2:D:701:FAD:H6	1.74	0.69
1:A:51:GLN:HG2	1:A:52:ALA:N	2.07	0.69
1:B:468:LEU:HD22	1:B:475:LYS:HG3	1.74	0.68
1:D:337:MET:HG2	1:D:337:MET:O	1.94	0.67
1:C:358:TRP:O	1:C:604:MET:HG3	1.96	0.65
1:A:51:GLN:CB	2:A:701:FAD:H2'	2.27	0.64
1:D:141:PRO:HD2	2:D:701:FAD:H62A	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276[A]:GLU:OE1	3:D:802:HOH:O	2.16	0.63
2:D:701:FAD:N1	2:D:701:FAD:H2'	2.14	0.63
1:B:130:ALA:HB2	3:B:880:HOH:O	1.98	0.62
1:D:43:ARG:NE	2:D:701:FAD:O2B	2.31	0.62
1:D:51:GLN:HA	2:D:701:FAD:C10	2.30	0.62
1:D:50:GLY:C	1:D:51:GLN:HG3	2.20	0.62
1:C:301:THR:HG21	2:C:701:FAD:H6	1.82	0.61
1:D:522:SER:OG	1:D:540:PHE:HB3	2.01	0.61
1:B:79:MET:CE	1:B:243:PRO:HD2	2.30	0.60
1:C:522:SER:OG	1:C:540:PHE:HB3	2.02	0.60
1:C:88:SER:HB3	1:C:92:GLY:O	2.02	0.60
1:C:155:ASP:O	1:C:318:ARG:NH2	2.34	0.60
1:B:155:ASP:O	1:B:318:ARG:NH2	2.35	0.60
1:A:88:SER:HB3	1:A:92:GLY:O	2.02	0.59
1:A:155:ASP:O	1:A:318:ARG:NH2	2.35	0.59
1:D:21:PRO:CB	1:D:337:MET:HG3	2.33	0.59
1:A:522:SER:OG	1:A:540:PHE:HB3	2.03	0.58
1:D:155:ASP:O	1:D:318:ARG:NH2	2.36	0.58
1:B:522:SER:OG	1:B:540:PHE:HB3	2.04	0.57
1:D:88:SER:HB3	1:D:92:GLY:O	2.04	0.57
1:B:79:MET:HE3	1:B:242:ILE:HG23	1.87	0.57
1:B:88:SER:HB3	1:B:92:GLY:O	2.03	0.57
1:C:522:SER:HB2	3:C:830:HOH:O	2.05	0.56
1:B:79:MET:HE3	1:B:114:THR:HG21	1.86	0.56
1:D:41:ASP:HA	2:D:701:FAD:N3A	2.21	0.55
1:A:51:GLN:OE1	2:A:701:FAD:H4'	2.06	0.55
1:A:51:GLN:HG3	2:A:701:FAD:C2	2.36	0.54
1:C:183:LYS:O	1:C:318:ARG:NH1	2.41	0.53
1:A:48:ALA:O	1:A:116:HIS:ND1	2.41	0.53
1:D:43:ARG:NH2	3:D:806:HOH:O	2.41	0.53
1:A:183:LYS:O	1:A:318:ARG:NH1	2.38	0.53
1:B:183:LYS:O	1:B:318:ARG:NH1	2.41	0.53
1:A:51:GLN:HG3	2:A:701:FAD:O2	2.10	0.52
1:A:21:PRO:HB3	1:A:337:MET:HE2	1.90	0.52
1:D:183:LYS:O	1:D:318:ARG:NH1	2.40	0.52
1:B:79:MET:HE2	1:B:243:PRO:HG2	1.91	0.52
1:C:337:MET:CE	1:C:341:MET:SD	2.98	0.52
1:C:255:LEU:HD12	1:C:302:LEU:HD21	1.92	0.52
1:D:58:ARG:NH1	1:D:447:ARG:HG3	2.25	0.51
2:D:701:FAD:O2'	2:D:701:FAD:O4'	2.26	0.51
1:A:265:THR:CB	1:A:267:ARG:HH11	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ALA:O	1:D:116:HIS:ND1	2.44	0.50
1:C:166:LYS:HB2	3:C:891:HOH:O	2.12	0.50
1:B:58:ARG:NH1	1:B:447:ARG:HG3	2.28	0.48
2:B:701:FAD:H9	2:B:701:FAD:H1'1	1.69	0.48
1:B:53:ASP:O	1:B:114:THR:HA	2.14	0.48
1:D:21:PRO:CG	1:D:337:MET:HG3	2.44	0.48
1:D:43:ARG:NH1	3:D:806:HOH:O	2.46	0.48
1:A:43:ARG:NH1	1:A:47:VAL:HG13	2.22	0.47
1:A:102:VAL:O	1:C:555:TYR:OH	2.29	0.47
1:A:522:SER:HB2	3:A:808:HOH:O	2.14	0.47
1:C:603:PHE:CE2	1:C:604:MET:HE2	2.50	0.47
1:B:402:VAL:HG12	1:B:406:GLU:HB2	1.95	0.47
1:C:166:LYS:HD2	3:C:891:HOH:O	2.14	0.47
1:B:79:MET:CE	1:B:242:ILE:HG23	2.44	0.47
2:C:701:FAD:H9	2:C:701:FAD:H1'1	1.67	0.46
1:B:260:VAL:CG1	1:B:260:VAL:O	2.63	0.46
1:C:511:HIS:O	1:C:512:GLU:HB2	2.15	0.46
1:A:26:CYS:HB2	1:A:344:THR:HB	1.98	0.46
1:C:276:GLU:OE2	1:D:287:LYS:NZ	2.43	0.46
1:C:53:ASP:O	1:C:114:THR:HA	2.15	0.46
1:D:50:GLY:C	1:D:51:GLN:CG	2.83	0.46
1:A:51:GLN:CB	2:A:701:FAD:C10	2.75	0.46
3:A:869:HOH:O	1:C:78:GLN:HB2	2.16	0.46
1:C:22:ALA:HB2	1:C:340:SER:OG	2.15	0.46
1:C:603:PHE:CE2	1:C:604:MET:CE	2.99	0.45
1:D:79:MET:HG3	1:D:243:PRO:HG2	1.99	0.45
1:D:53:ASP:O	1:D:114:THR:HA	2.17	0.44
1:D:493:ALA:O	1:D:497:GLU:HG2	2.17	0.44
1:B:267:ARG:HA	1:B:267:ARG:NH2	2.32	0.44
1:A:53:ASP:O	1:A:114:THR:HA	2.16	0.44
1:D:59:THR:CG2	1:D:341:MET:CE	2.95	0.44
1:A:265:THR:CB	1:A:267:ARG:NH1	2.80	0.44
1:B:255:LEU:HD12	1:B:302:LEU:HD21	1.99	0.44
1:D:358:TRP:O	1:D:604:MET:HG3	2.18	0.44
1:B:56:GLN:CD	1:B:418:THR:O	2.56	0.44
1:D:41:ASP:HA	2:D:701:FAD:C2A	2.48	0.43
1:D:235:HIS:CE1	1:D:236:ASN:CB	2.94	0.43
1:B:5:ILE:HG22	1:B:175:SER:HB2	2.00	0.43
1:C:236:ASN:HD22	1:C:284:GLU:HB3	1.83	0.43
1:A:301:THR:HG21	2:A:701:FAD:N5	2.34	0.43
1:B:260:VAL:O	1:B:260:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:HIS:HB2	3:D:818:HOH:O	2.18	0.43
1:A:51:GLN:CB	2:A:701:FAD:C2	2.97	0.42
1:B:79:MET:HE1	1:B:242:ILE:HA	2.01	0.42
1:A:51:GLN:CG	2:A:701:FAD:C2	2.97	0.42
1:A:321:ILE:HD12	1:A:326:CYS:HB3	2.00	0.42
1:C:321:ILE:HD12	1:C:326:CYS:HB3	2.01	0.42
1:D:50:GLY:HA3	1:D:299:TRP:CZ2	2.55	0.42
1:D:26:CYS:HB2	1:D:344:THR:HB	2.00	0.42
1:D:234:SER:OG	1:D:236:ASN:OD1	2.38	0.42
1:A:236:ASN:HD22	1:A:284:GLU:HB3	1.85	0.42
1:C:273:VAL:HB	1:C:302:LEU:HD11	2.02	0.42
1:D:51:GLN:HA	2:D:701:FAD:C4	2.49	0.41
1:D:511:HIS:O	1:D:512:GLU:HB2	2.20	0.41
1:B:511:HIS:O	1:B:512:GLU:HB2	2.20	0.41
1:D:21:PRO:HB3	1:D:337:MET:HG3	2.01	0.41
1:A:511:HIS:O	1:A:512:GLU:HB2	2.20	0.41
1:A:52:ALA:CB	1:A:337:MET:HG2	2.51	0.41
1:B:434:LYS:HB2	1:B:434:LYS:HE3	1.94	0.41
1:B:329:HIS:HB2	3:B:871:HOH:O	2.20	0.40
1:C:26:CYS:HB2	1:C:344:THR:HB	2.02	0.40
1:D:50:GLY:O	1:D:117:GLN:HB2	2.20	0.40
1:D:337:MET:HB2	2:D:701:FAD:H4'	2.03	0.40
1:D:321:ILE:HD12	1:D:326:CYS:HB3	2.03	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	601/624 (96%)	577 (96%)	24 (4%)	0	100	100
1	B	601/624 (96%)	581 (97%)	20 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	600/624 (96%)	575 (96%)	25 (4%)	0	100 100
1	D	601/624 (96%)	577 (96%)	23 (4%)	1 (0%)	44 58
All	All	2403/2496 (96%)	2310 (96%)	92 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	51	GLN

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	488/507 (96%)	475 (97%)	13 (3%)	40 58
1	B	488/507 (96%)	479 (98%)	9 (2%)	54 72
1	C	487/507 (96%)	476 (98%)	11 (2%)	45 64
1	D	488/507 (96%)	475 (97%)	13 (3%)	40 58
All	All	1951/2028 (96%)	1905 (98%)	46 (2%)	44 63

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	SER
1	A	103	THR
1	A	129	LYS
1	A	258	ARG
1	A	312	ARG
1	A	314	SER
1	A	337	MET
1	A	412	GLN
1	A	447	ARG
1	A	475	LYS
1	A	513	ASN

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Mol	Chain	Res	Type
1	A	533	TYR
1	A	594	ARG
1	B	88	SER
1	B	103	THR
1	B	106	ASN
1	B	314	SER
1	B	387	LYS
1	B	447	ARG
1	B	475	LYS
1	B	513	ASN
1	B	594	ARG
1	C	8	LYS
1	C	88	SER
1	C	106	ASN
1	C	129	LYS
1	C	137	ARG
1	C	260	VAL
1	C	314	SER
1	C	412	GLN
1	C	447	ARG
1	C	475	LYS
1	C	604	MET
1	D	79	MET
1	D	88	SER
1	D	103	THR
1	D	137	ARG
1	D	236	ASN
1	D	258	ARG
1	D	261	LEU
1	D	337	MET
1	D	412	GLN
1	D	447	ARG
1	D	475	LYS
1	D	528	LYS
1	D	604	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	ASN
1	B	513	ASN
1	C	207	GLN

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Mol	Chain	Res	Type
1	C	432	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	701	-	53,58,58	0.86	2 (3%)	68,89,89	1.11	5 (7%)
2	FAD	A	701	-	53,58,58	1.27	3 (5%)	68,89,89	1.59	9 (13%)
2	FAD	C	701	-	53,58,58	0.78	1 (1%)	68,89,89	1.07	5 (7%)
2	FAD	B	701	-	53,58,58	0.85	1 (1%)	68,89,89	1.06	4 (5%)

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	D	701	-	-	15/30/50/50	0/6/6/6
2	FAD	A	701	-	-	19/30/50/50	0/6/6/6
2	FAD	C	701	-	-	15/30/50/50	0/6/6/6
2	FAD	B	701	-	-	5/30/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAD	C1'-C2'	4.70	1.59	1.52
2	A	701	FAD	C2-N3	-3.39	1.31	1.39
2	C	701	FAD	C1'-C2'	-3.13	1.48	1.52
2	A	701	FAD	C10-N10	2.76	1.43	1.37
2	B	701	FAD	C1'-C2'	-2.73	1.48	1.52
2	D	701	FAD	C4X-C4	-2.11	1.36	1.44
2	D	701	FAD	C10-N10	2.02	1.41	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FAD	P-O3P-PA	6.16	153.97	132.83
2	A	701	FAD	O5'-C5'-C4'	5.73	124.66	109.36
2	D	701	FAD	O5'-C5'-C4'	4.00	120.04	109.36
2	D	701	FAD	P-O3P-PA	3.94	146.35	132.83
2	B	701	FAD	P-O3P-PA	3.85	146.03	132.83
2	A	701	FAD	C1'-C2'-C3'	3.81	120.45	109.79
2	C	701	FAD	C1'-C2'-C3'	-3.15	100.98	109.79
2	C	701	FAD	O5'-P-O1P	-3.01	97.31	109.07
2	A	701	FAD	C5'-C4'-C3'	2.95	117.90	112.20
2	B	701	FAD	O2'-C2'-C3'	2.74	115.75	109.10
2	D	701	FAD	O4-C4-C4X	-2.65	119.58	126.60
2	C	701	FAD	O2P-P-O1P	2.61	125.15	112.24
2	A	701	FAD	C4-N3-C2	-2.54	120.95	125.64
2	A	701	FAD	C4X-C4-N3	2.52	119.59	113.19
2	B	701	FAD	C1'-C2'-C3'	-2.46	102.92	109.79
2	C	701	FAD	C1'-N10-C9A	-2.42	116.48	120.51
2	D	701	FAD	C4X-C4-N3	2.35	119.17	113.19
2	C	701	FAD	C4-N3-C2	-2.34	121.32	125.64
2	B	701	FAD	C5A-C6A-N6A	2.31	123.87	120.35
2	A	701	FAD	C9-C9A-N10	2.20	124.81	121.84
2	A	701	FAD	O2-C2-N3	-2.06	114.64	118.65
2	D	701	FAD	C4-N3-C2	-2.05	121.85	125.64
2	A	701	FAD	C4A-C5A-N7A	2.04	111.52	109.40

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5B-O5B-PA-O1A
2	A	701	FAD	C5B-O5B-PA-O2A
2	A	701	FAD	C1'-C2'-C3'-O3'
2	A	701	FAD	C1'-C2'-C3'-C4'
2	A	701	FAD	C2'-C3'-C4'-O4'
2	A	701	FAD	C2'-C3'-C4'-C5'
2	A	701	FAD	O3'-C3'-C4'-O4'
2	A	701	FAD	O3'-C3'-C4'-C5'
2	A	701	FAD	C3'-C4'-C5'-O5'
2	A	701	FAD	PA-O3P-P-O5'
2	B	701	FAD	C3'-C4'-C5'-O5'
2	B	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	C5B-O5B-PA-O2A
2	C	701	FAD	C2'-C3'-C4'-O4'
2	C	701	FAD	C2'-C3'-C4'-C5'
2	C	701	FAD	O3'-C3'-C4'-O4'
2	C	701	FAD	O3'-C3'-C4'-C5'
2	C	701	FAD	O4'-C4'-C5'-O5'
2	D	701	FAD	C5B-O5B-PA-O1A
2	D	701	FAD	C5B-O5B-PA-O2A
2	D	701	FAD	C2'-C1'-N10-C10
2	D	701	FAD	N10-C1'-C2'-O2'
2	D	701	FAD	N10-C1'-C2'-C3'
2	D	701	FAD	C2'-C3'-C4'-O4'
2	D	701	FAD	C2'-C3'-C4'-C5'
2	D	701	FAD	C3'-C4'-C5'-O5'
2	D	701	FAD	O4'-C4'-C5'-O5'
2	A	701	FAD	O2'-C2'-C3'-O3'
2	D	701	FAD	O3'-C3'-C4'-O4'
2	A	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	C3B-C4B-C5B-O5B
2	C	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	C3B-C4B-C5B-O5B
2	D	701	FAD	O3'-C3'-C4'-C5'
2	C	701	FAD	C3B-C4B-C5B-O5B
2	A	701	FAD	C4B-C5B-O5B-PA
2	C	701	FAD	C3'-C4'-C5'-O5'
2	D	701	FAD	C4B-C5B-O5B-PA

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Mol	Chain	Res	Type	Atoms
2	C	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	C5B-O5B-PA-O3P
2	D	701	FAD	C5B-O5B-PA-O3P
2	A	701	FAD	O2'-C2'-C3'-C4'
2	A	701	FAD	O4'-C4'-C5'-O5'
2	A	701	FAD	C5B-O5B-PA-O3P
2	C	701	FAD	C5'-O5'-P-O3P
2	A	701	FAD	P-O3P-PA-O1A
2	A	701	FAD	P-O3P-PA-O2A
2	B	701	FAD	PA-O3P-P-O1P
2	C	701	FAD	PA-O3P-P-O1P
2	C	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	N10-C1'-C2'-O2'

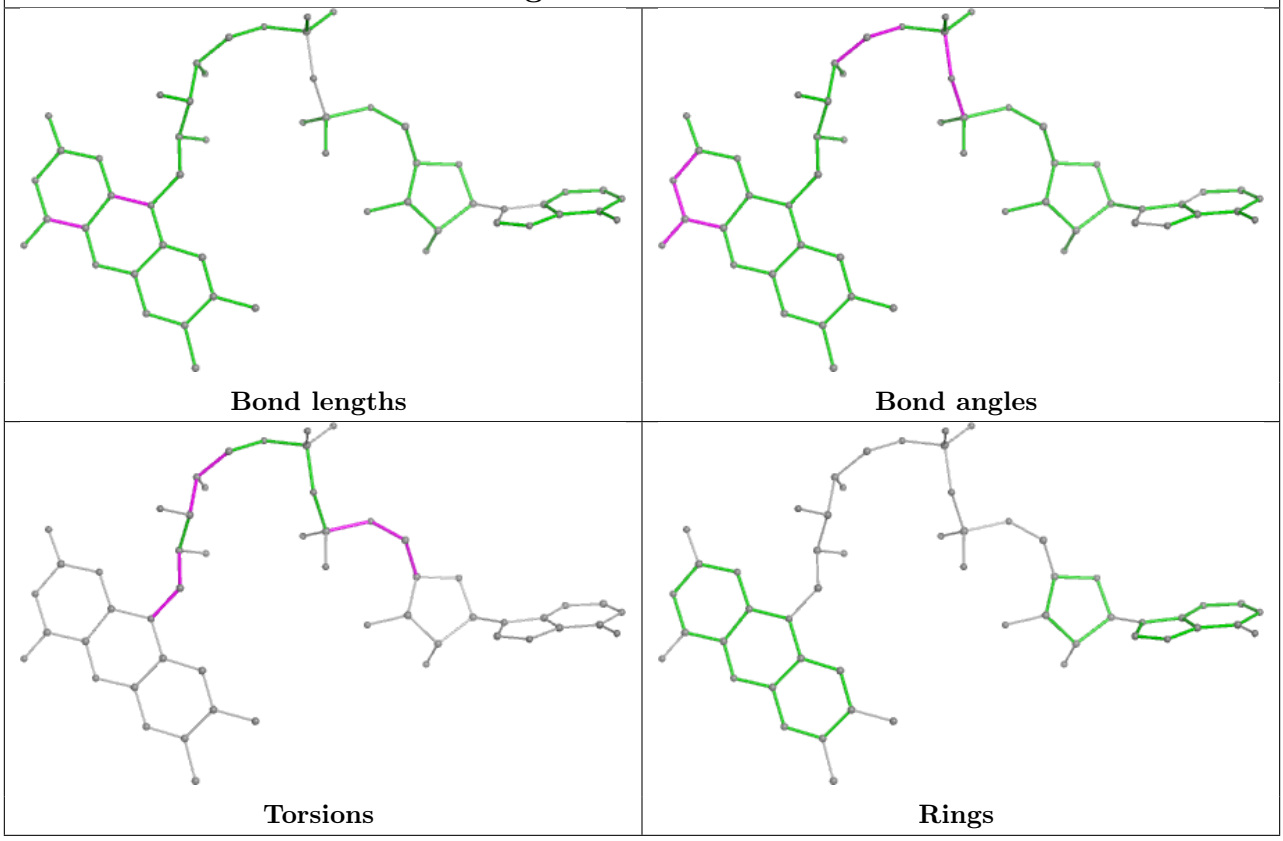
There are no ring outliers.

4 monomers are involved in 26 short contacts:

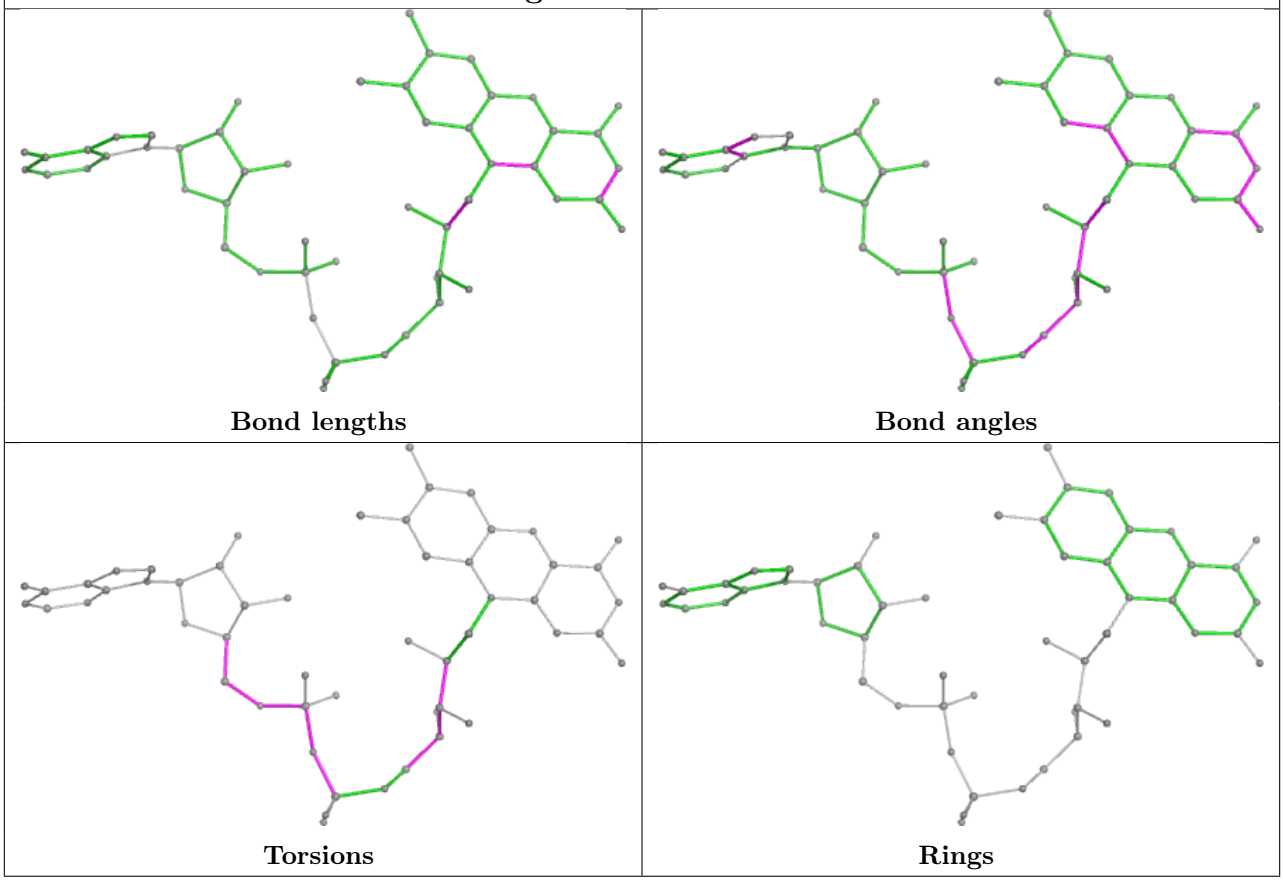
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	FAD	11	0
2	A	701	FAD	12	0
2	C	701	FAD	2	0
2	B	701	FAD	1	0

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 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.

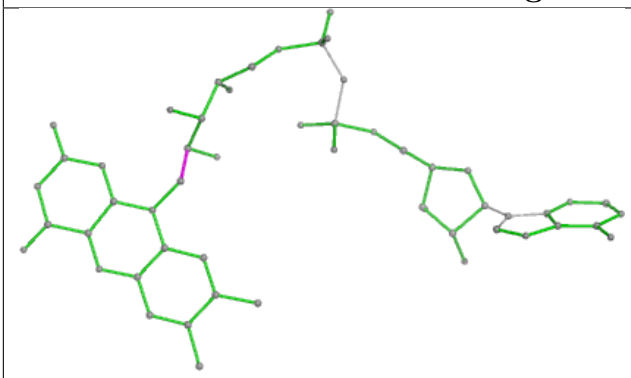
Ligand FAD D 701



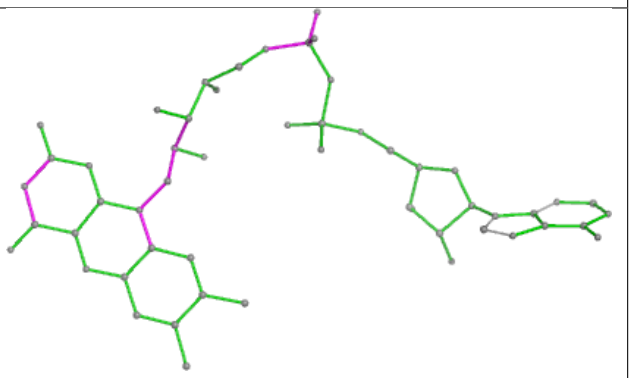
Ligand FAD A 701



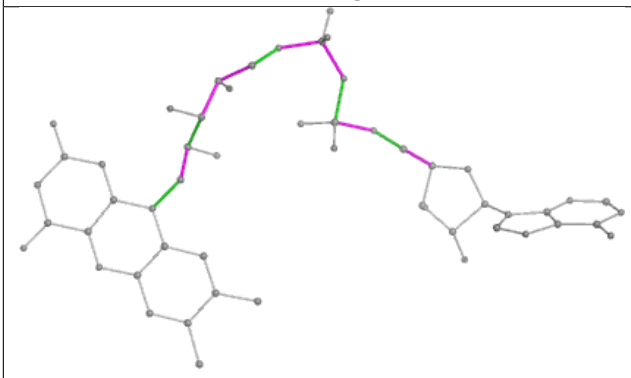
Ligand FAD C 701



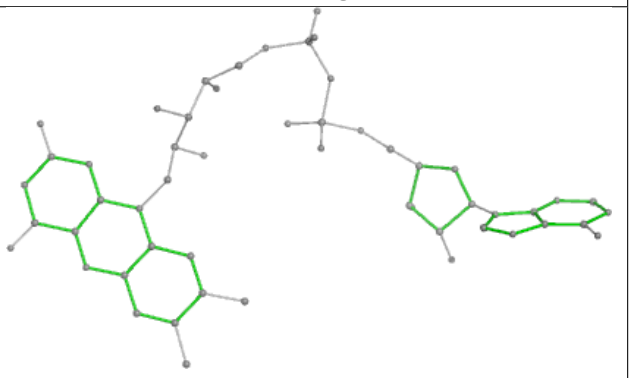
Bond lengths



Bond angles

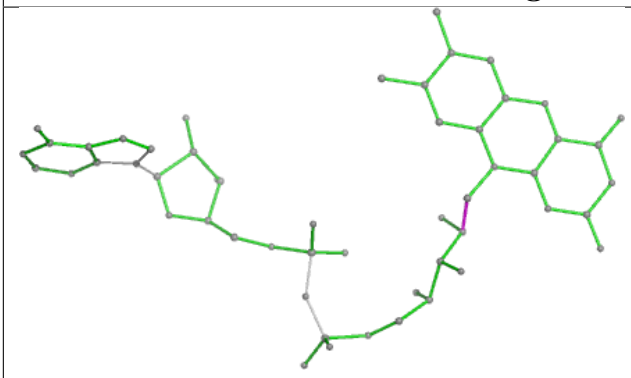


Torsions

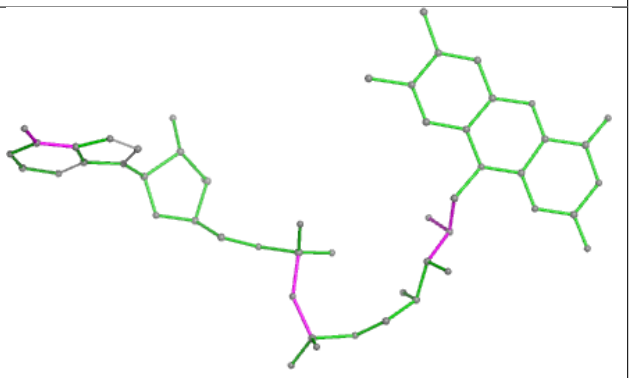


Rings

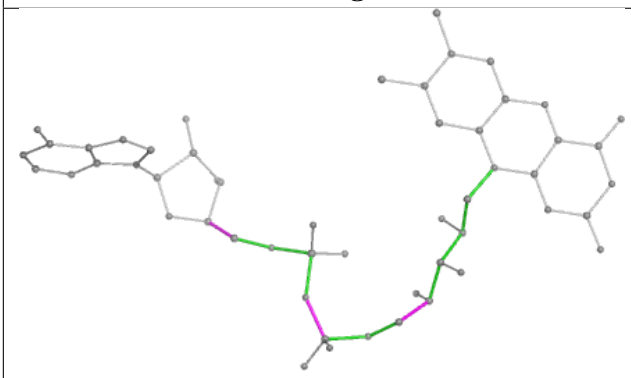
Ligand FAD B 701



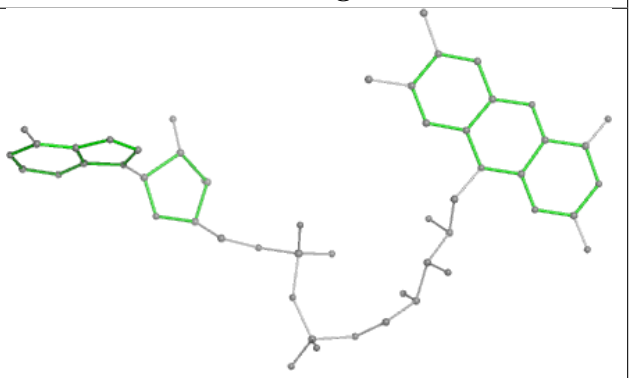
Bond lengths



Bond angles



Torsions



Rings

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	602/624 (96%)	-0.29	22 (3%)	45	43	11, 21, 57, 104	1 (0%)
1	B	602/624 (96%)	-0.25	17 (2%)	55	52	11, 21, 61, 114	1 (0%)
1	C	602/624 (96%)	-0.25	18 (2%)	52	50	10, 23, 59, 103	0
1	D	602/624 (96%)	-0.26	21 (3%)	47	45	10, 23, 54, 99	1 (0%)
All	All	2408/2496 (96%)	-0.27	78 (3%)	50	47	10, 22, 59, 114	3 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	606	ALA	7.2
1	A	5	ILE	7.1
1	C	606	ALA	6.7
1	B	606	ALA	5.8
1	A	173	GLY	5.7
1	A	606	ALA	5.4
1	C	264	ALA	5.4
1	B	265	THR	5.1
1	B	264	ALA	5.0
1	A	172	ALA	4.8
1	D	5	ILE	4.6
1	D	173	GLY	4.6
1	A	237	GLY	4.6
1	D	172	ALA	4.4
1	D	264	ALA	4.3
1	C	265	THR	4.2
1	C	404	HIS	3.9
1	A	268	VAL	3.8
1	C	397	ASP	3.7
1	D	268	VAL	3.7
1	C	266	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	263	PRO	3.6
1	A	265	THR	3.6
1	C	5	ILE	3.6
1	B	268	VAL	3.6
1	C	268	VAL	3.6
1	A	264	ALA	3.5
1	B	5	ILE	3.5
1	B	263	PRO	3.4
1	B	397	ASP	3.4
1	C	263	PRO	3.3
1	A	235	HIS	3.2
1	D	267	ARG	3.2
1	A	236	ASN	3.1
1	A	261	LEU	3.1
1	B	267	ARG	3.0
1	A	263	PRO	2.9
1	A	171	PRO	2.9
1	C	267	ARG	2.7
1	D	171	PRO	2.7
1	B	236	ASN	2.7
1	B	395	THR	2.7
1	C	395	THR	2.7
1	B	266	GLY	2.7
1	B	235	HIS	2.6
1	B	171	PRO	2.6
1	C	398	ASN	2.6
1	A	174	GLN	2.6
1	A	267	ARG	2.6
1	C	270	LYS	2.6
1	D	236	ASN	2.6
1	D	174	GLN	2.6
1	B	404	HIS	2.6
1	D	237	GLY	2.6
1	D	47	VAL	2.5
1	C	605	ALA	2.5
1	A	6	ALA	2.5
1	B	172	ALA	2.5
1	A	47	VAL	2.5
1	D	6	ALA	2.4
1	C	173	GLY	2.4
1	A	106	ASN	2.4
1	D	238	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	384	LYS	2.3
1	A	51	GLN	2.3
1	D	48	ALA	2.3
1	C	396	GLU	2.2
1	D	46	LYS	2.2
1	A	266	GLY	2.2
1	C	174	GLN	2.2
1	D	233	HIS	2.2
1	D	265	THR	2.1
1	A	513	ASN	2.1
1	A	45	VAL	2.1
1	C	172	ALA	2.1
1	D	235	HIS	2.1
1	D	384	LYS	2.1
1	B	258	ARG	2.0

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)

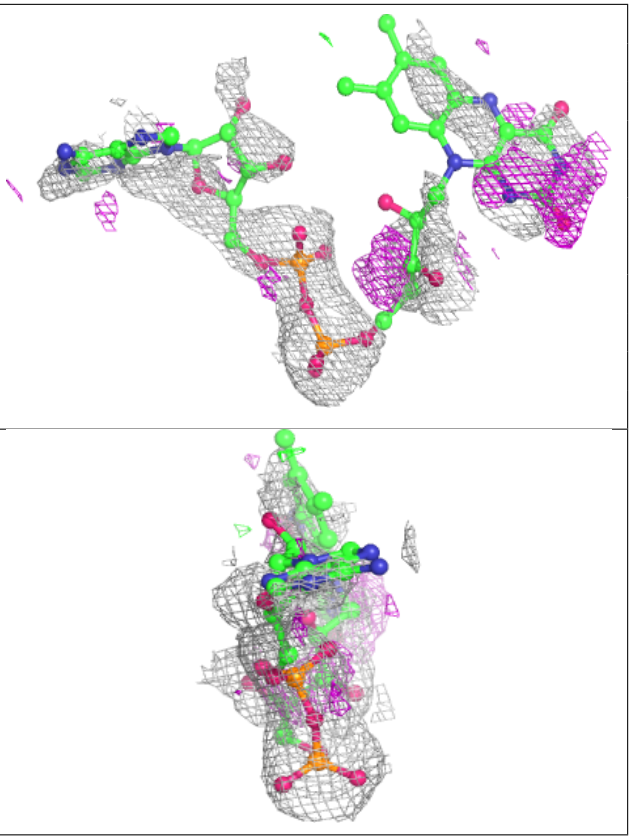
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A	701	53/53	0.86	0.24	29,103,137,145	0
2	FAD	D	701	53/53	0.87	0.21	31,79,113,122	0
2	FAD	C	701	53/53	0.95	0.09	22,36,42,43	0
2	FAD	B	701	53/53	0.95	0.09	22,37,51,52	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.

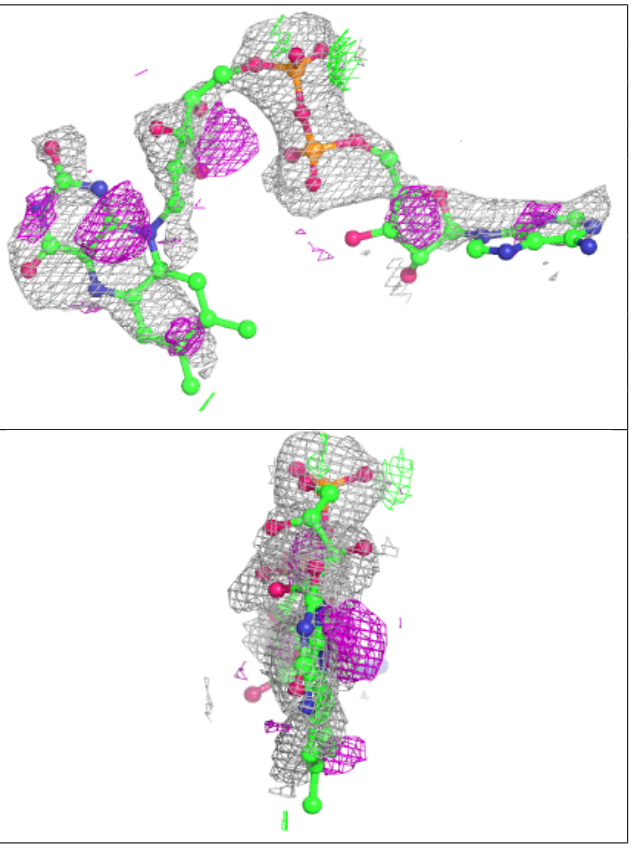
Electron density around FAD A 701:

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



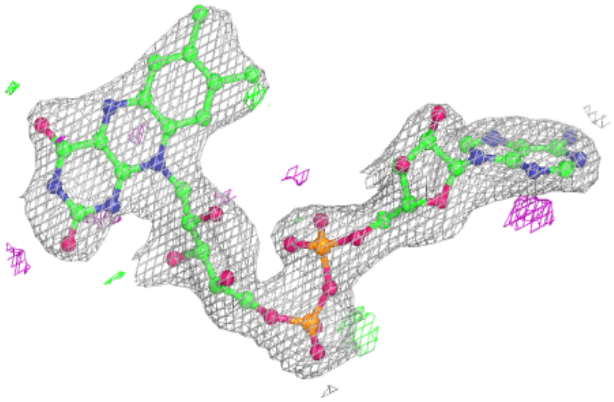
Electron density around FAD D 701:

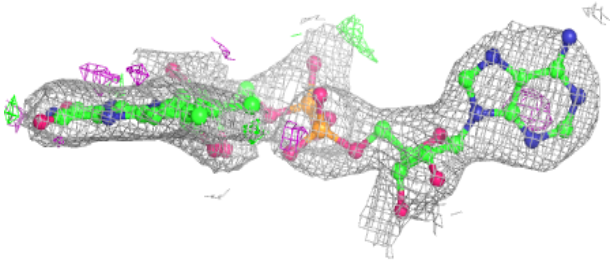
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

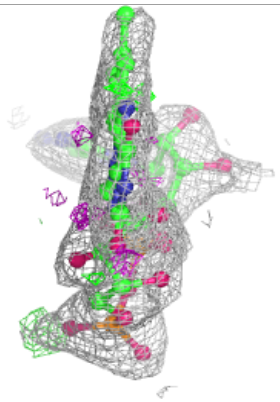


Electron density around FAD C 701:

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

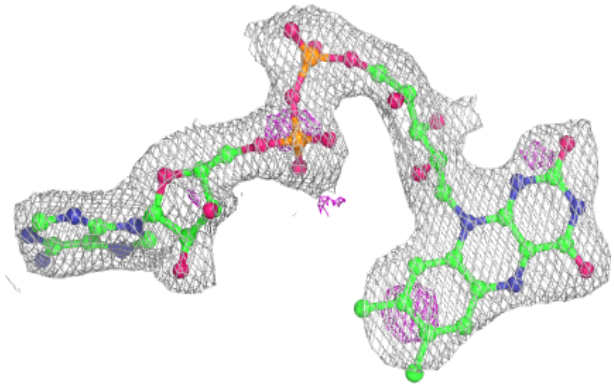


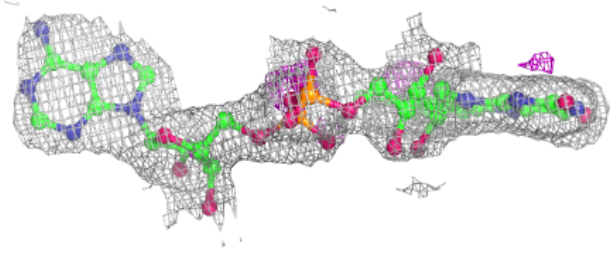


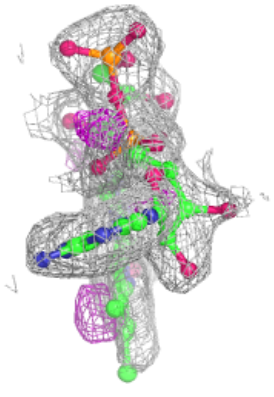


Electron density around FAD B 701:

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







6.5 Other polymers (i)

There are no such residues in this entry.