



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:03 am BST

PDB ID : 4F8Y
Title : Complex structure of NADPH:quinone oxidoreductase with menadione in Streptococcus mutans
Authors : Wang, Z.; Li, L.; Su, X.-D.
Deposited on : 2012-05-18
Resolution : 1.80 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 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 : 2.11
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) : 2.11

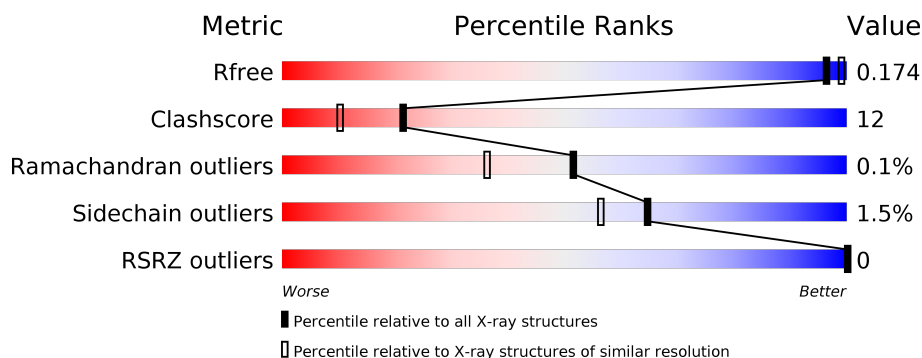
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	196	<div> <div>79%</div> <div>21%</div> </div>
1	B	196	<div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	C	196	<div> <div>79%</div> <div>21%</div> <div>•</div> </div>
1	D	196	<div> <div>74%</div> <div>19%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	VK3	C	202	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6966 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 NADPH Quinone Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1577	1026	267	279	5			
1	B	188	Total	C	N	O	S	0	0	0
			1506	982	248	271	5			
1	C	196	Total	C	N	O	S	0	0	0
			1572	1022	266	279	5			
1	D	188	Total	C	N	O	S	0	0	0
			1489	972	246	266	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	LEU	-	EXPRESSION TAG	UNP Q8DTD1
A	190	GLU	-	EXPRESSION TAG	UNP Q8DTD1
A	191	HIS	-	EXPRESSION TAG	UNP Q8DTD1
A	192	HIS	-	EXPRESSION TAG	UNP Q8DTD1
A	193	HIS	-	EXPRESSION TAG	UNP Q8DTD1
A	194	HIS	-	EXPRESSION TAG	UNP Q8DTD1
A	195	HIS	-	EXPRESSION TAG	UNP Q8DTD1
A	196	HIS	-	EXPRESSION TAG	UNP Q8DTD1
B	189	LEU	-	EXPRESSION TAG	UNP Q8DTD1
B	190	GLU	-	EXPRESSION TAG	UNP Q8DTD1
B	191	HIS	-	EXPRESSION TAG	UNP Q8DTD1
B	192	HIS	-	EXPRESSION TAG	UNP Q8DTD1
B	193	HIS	-	EXPRESSION TAG	UNP Q8DTD1
B	194	HIS	-	EXPRESSION TAG	UNP Q8DTD1
B	195	HIS	-	EXPRESSION TAG	UNP Q8DTD1
B	196	HIS	-	EXPRESSION TAG	UNP Q8DTD1
C	189	LEU	-	EXPRESSION TAG	UNP Q8DTD1
C	190	GLU	-	EXPRESSION TAG	UNP Q8DTD1
C	191	HIS	-	EXPRESSION TAG	UNP Q8DTD1
C	192	HIS	-	EXPRESSION TAG	UNP Q8DTD1
C	193	HIS	-	EXPRESSION TAG	UNP Q8DTD1

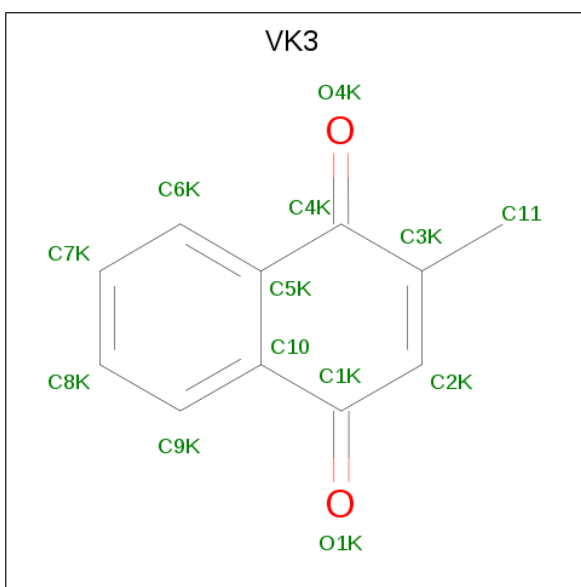
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Chain	Residue	Modelled	Actual	Comment	Reference
C	194	HIS	-	EXPRESSION TAG	UNP Q8DTD1
C	195	HIS	-	EXPRESSION TAG	UNP Q8DTD1
C	196	HIS	-	EXPRESSION TAG	UNP Q8DTD1
D	189	LEU	-	EXPRESSION TAG	UNP Q8DTD1
D	190	GLU	-	EXPRESSION TAG	UNP Q8DTD1
D	191	HIS	-	EXPRESSION TAG	UNP Q8DTD1
D	192	HIS	-	EXPRESSION TAG	UNP Q8DTD1
D	193	HIS	-	EXPRESSION TAG	UNP Q8DTD1
D	194	HIS	-	EXPRESSION TAG	UNP Q8DTD1
D	195	HIS	-	EXPRESSION TAG	UNP Q8DTD1
D	196	HIS	-	EXPRESSION TAG	UNP Q8DTD1

- # FAD

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	11	2		
3	B	1	Total	C	O	0	0
			13	11	2		
3	C	1	Total	C	O	0	0
			13	11	2		
3	D	1	Total	C	O	0	0
			13	11	2		

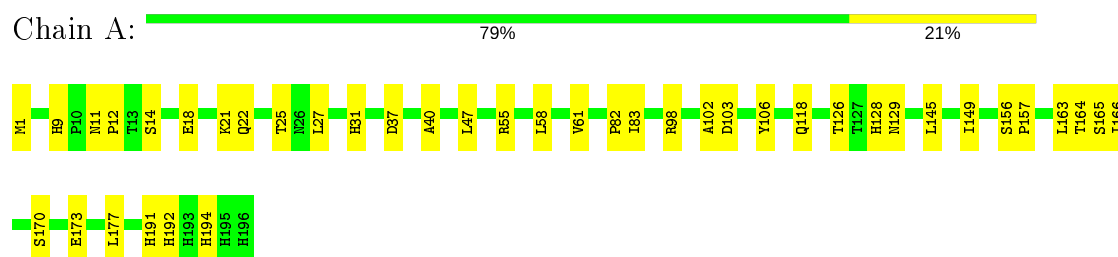
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	117	Total	O	0	0
			117	117		
4	C	172	Total	O	0	0
			172	172		
4	D	112	Total	O	0	0
			112	112		

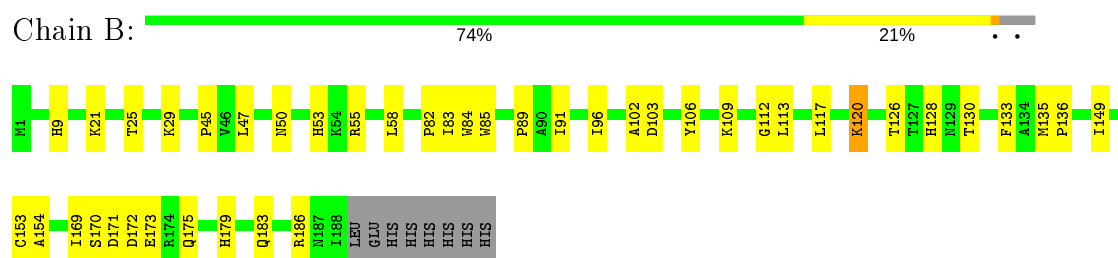
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

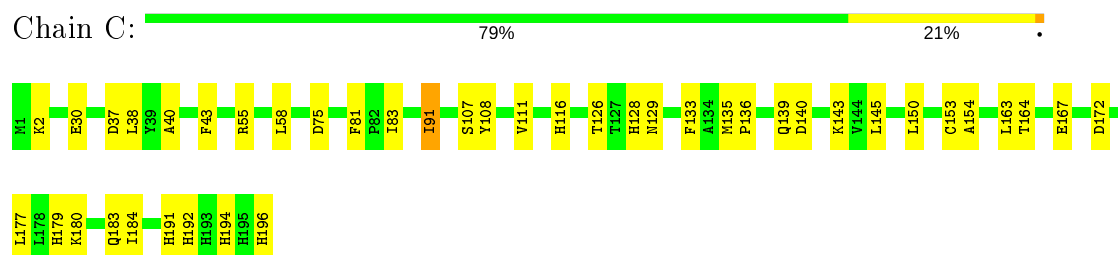
• Molecule 1: NADPH Quinone Oxidoreductase



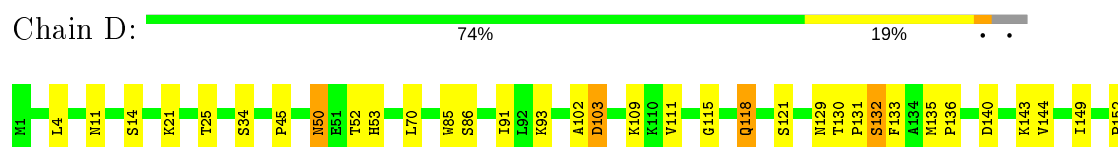
• Molecule 1: NADPH Quinone Oxidoreductase



• Molecule 1: NADPH Quinone Oxidoreductase



• Molecule 1: NADPH Quinone Oxidoreductase



P157	T164	S165	I166	E167	D172	E173	R174	K180	I184	I188	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.61Å 79.41Å 106.50Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	19.96 – 1.80 19.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.96-1.80) 98.0 (19.96-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.156 , 0.183 0.157 , 0.174	Depositor DCC
R_{free} test set	3897 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6966	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VK3, 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	0.33	0/1623	0.49	0/2209
1	B	0.34	0/1546	0.52	0/2105
1	C	0.33	0/1618	0.50	0/2204
1	D	0.34	0/1528	0.50	0/2081
All	All	0.33	0/6315	0.50	0/8599

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1577	0	1541	34	0
1	B	1506	0	1490	38	0
1	C	1572	0	1528	41	0
1	D	1489	0	1471	30	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	13	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	8	4	0
3	C	13	0	8	6	0
3	D	13	0	8	5	0
4	A	157	0	0	5	0
4	B	117	0	0	7	0
4	C	172	0	0	17	0
4	D	112	0	0	4	0
All	All	6966	0	6186	151	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 12.

All (151) 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:C:191:HIS:CD2	1:C:192:HIS:HD2	1.82	0.98
1:C:129:ASN:HD21	1:C:167:GLU:HB2	1.29	0.93
1:B:50:ASN:HB2	4:B:354:HOH:O	1.67	0.92
1:C:191:HIS:HD2	1:C:192:HIS:HD2	1.13	0.92
1:C:129:ASN:HD21	1:C:167:GLU:CB	1.87	0.86
1:A:194:HIS:HE1	4:A:414:HOH:O	1.60	0.82
1:C:129:ASN:ND2	1:C:167:GLU:HB2	1.92	0.82
1:B:179:HIS:CE1	1:B:183:GLN:HE21	1.97	0.81
1:A:129:ASN:HD22	3:B:202:VK3:H7K1	1.45	0.81
1:C:191:HIS:HD2	1:C:192:HIS:CD2	1.98	0.81
1:C:38:LEU:HB3	1:C:91:ILE:HD12	1.62	0.79
4:C:443:HOH:O	3:D:202:VK3:H8K1	1.82	0.78
1:A:191:HIS:HD2	1:A:192:HIS:HD2	1.34	0.74
1:A:11:ASN:HA	1:B:50:ASN:HD21	1.54	0.72
1:A:1:MET:HB3	4:A:416:HOH:O	1.91	0.71
1:B:171:ASP:O	1:B:175:GLN:HG2	1.91	0.70
1:C:43:PHE:HB3	1:C:91:ILE:HD11	1.74	0.70
3:C:202:VK3:H113	4:C:463:HOH:O	1.91	0.69
3:D:202:VK3:H6K1	4:D:392:HOH:O	1.95	0.67
1:A:9:HIS:CD2	1:A:82:PRO:HG3	2.30	0.67
1:A:21:LYS:O	1:A:25:THR:HG23	1.94	0.67
1:D:50:ASN:ND2	1:D:52:THR:H	1.93	0.67
3:C:202:VK3:H6K1	4:C:433:HOH:O	1.95	0.66
1:A:11:ASN:HA	1:B:50:ASN:ND2	2.11	0.65
1:C:191:HIS:CD2	1:C:192:HIS:CD2	2.74	0.64
1:B:133:PHE:O	1:B:136:PRO:HD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLN:HE22	1:D:143:LYS:HB3	1.62	0.64
1:D:140:ASP:O	1:D:143:LYS:HE3	1.97	0.64
1:D:50:ASN:HD22	1:D:52:THR:H	1.44	0.64
1:A:106:TYR:OH	3:A:202:VK3:H9K1	1.99	0.63
1:B:126:THR:HB	4:B:397:HOH:O	1.99	0.63
1:C:91:ILE:HD13	1:C:91:ILE:O	2.00	0.62
1:D:21:LYS:O	1:D:25:THR:HG23	2.00	0.62
1:C:38:LEU:HB3	1:C:91:ILE:CD1	2.30	0.61
1:D:129:ASN:OD1	1:D:167:GLU:HB2	2.00	0.61
1:C:143:LYS:HE2	4:C:331:HOH:O	2.00	0.61
1:A:9:HIS:HD2	1:A:82:PRO:HG3	1.66	0.60
1:C:83:ILE:HB	1:C:128:HIS:HB3	1.84	0.60
1:B:96:ILE:HG21	1:B:149:ILE:HD13	1.83	0.60
1:A:191:HIS:CD2	1:A:192:HIS:HD2	2.19	0.60
1:A:11:ASN:HB3	1:A:14:SER:HB3	1.82	0.59
1:B:135:MET:HB3	4:B:401:HOH:O	2.02	0.59
1:D:11:ASN:HB3	1:D:14:SER:HB3	1.84	0.59
1:D:135:MET:HE2	1:D:135:MET:HA	1.83	0.59
1:A:102:ALA:O	1:A:103:ASP:HB2	2.02	0.59
3:A:202:VK3:H2K1	1:B:85:TRP:CZ3	2.38	0.58
1:A:129:ASN:HD22	3:B:202:VK3:C7K	2.17	0.57
1:C:128:HIS:CE1	1:C:164:THR:HG22	2.40	0.57
2:A:201:FAD:H9	1:B:55:ARG:NH1	2.21	0.56
4:A:303:HOH:O	2:B:201:FAD:HM72	2.05	0.55
1:B:170:SER:OG	1:B:173:GLU:HG3	2.07	0.55
1:B:9:HIS:HD2	1:B:82:PRO:HG3	1.72	0.55
3:C:202:VK3:H112	4:C:447:HOH:O	2.05	0.55
1:D:50:ASN:HD22	1:D:50:ASN:C	2.11	0.54
1:B:169:ILE:HB	1:B:173:GLU:CD	2.28	0.54
1:C:55:ARG:O	1:C:58:LEU:HG	2.08	0.54
1:D:50:ASN:HD22	1:D:52:THR:N	2.05	0.53
1:D:93:LYS:HE2	4:D:321:HOH:O	2.09	0.53
1:D:180:LYS:O	1:D:184:ILE:HG13	2.09	0.53
1:A:12:PRO:HD3	1:B:50:ASN:HD21	1.74	0.52
1:A:18:GLU:O	1:A:22:GLN:HG2	2.10	0.52
1:B:83:ILE:HB	1:B:128:HIS:HB3	1.92	0.52
1:D:164:THR:HG21	4:D:396:HOH:O	2.08	0.52
1:C:129:ASN:ND2	1:C:167:GLU:OE1	2.44	0.51
1:B:45:PRO:HB3	1:B:91:ILE:HA	1.93	0.51
1:D:130:THR:CG2	1:D:135:MET:HE3	2.42	0.50
1:A:83:ILE:HB	1:A:128:HIS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:HIS:HE1	4:C:301:HOH:O	1.95	0.50
1:C:108:TYR:HE2	3:C:202:VK3:C7K	2.25	0.49
2:C:201:FAD:H8A	4:C:424:HOH:O	2.11	0.49
1:D:4:LEU:HD13	1:D:70:LEU:HD22	1.94	0.49
1:D:102:ALA:O	1:D:103:ASP:HB2	2.11	0.49
1:D:131:PRO:HB3	1:D:133:PHE:CE1	2.47	0.49
1:B:106:TYR:CD2	1:B:113:LEU:HD22	2.46	0.49
1:B:130:THR:CG2	1:B:135:MET:HE3	2.42	0.49
1:C:179:HIS:O	1:C:183:GLN:HG3	2.12	0.49
1:A:194:HIS:HD2	4:A:424:HOH:O	1.95	0.49
1:C:58:LEU:HB2	4:C:318:HOH:O	2.12	0.48
1:B:130:THR:HG21	1:B:135:MET:CE	2.44	0.48
1:D:132:SER:HB3	4:D:396:HOH:O	2.14	0.48
1:D:50:ASN:HD21	1:D:53:HIS:H	1.62	0.48
1:D:132:SER:HA	1:D:135:MET:HG2	1.96	0.48
2:A:201:FAD:HM72	4:B:306:HOH:O	2.13	0.47
1:B:53:HIS:HD2	4:B:395:HOH:O	1.98	0.47
1:C:135:MET:N	1:C:136:PRO:CD	2.78	0.47
1:B:117:LEU:O	1:B:120:LYS:HB2	2.15	0.47
1:C:180:LYS:O	1:C:184:ILE:HG13	2.14	0.47
1:A:129:ASN:ND2	3:B:202:VK3:H7K1	2.23	0.46
1:C:2:LYS:HE3	1:C:75:ASP:OD2	2.15	0.46
1:C:133:PHE:HD1	4:C:411:HOH:O	1.99	0.46
1:C:194:HIS:HD2	4:C:385:HOH:O	1.98	0.46
1:B:135:MET:HA	1:B:135:MET:HE2	1.98	0.46
1:D:45:PRO:HB3	1:D:91:ILE:HA	1.98	0.46
1:D:85:TRP:O	1:D:86:SER:HB2	2.16	0.46
1:A:47:LEU:HD13	1:A:98:ARG:HA	1.98	0.46
1:C:163:LEU:HB3	1:C:177:LEU:HD13	1.97	0.46
1:B:109:LYS:HZ1	1:B:112:GLY:H	1.64	0.45
1:B:126:THR:CB	4:B:397:HOH:O	2.62	0.45
1:C:30:GLU:HG3	1:C:196:HIS:ND1	2.32	0.45
1:C:37:ASP:HB3	1:C:40:ALA:HB3	1.97	0.45
1:C:153:CYS:O	1:C:154:ALA:HB3	2.16	0.45
4:C:427:HOH:O	3:D:202:VK3:H111	2.17	0.45
1:B:183:GLN:CD	1:B:186:ARG:HH12	2.18	0.45
1:C:107:SER:OG	1:C:116:HIS:CE1	2.70	0.45
1:B:106:TYR:CD2	1:B:106:TYR:C	2.90	0.45
1:C:81:PHE:O	1:C:126:THR:HA	2.17	0.45
1:A:145:LEU:HA	1:A:149:ILE:HD12	1.98	0.44
1:A:37:ASP:HB3	1:A:40:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LYS:O	1:B:25:THR:HG23	2.16	0.44
1:B:84:TRP:CZ3	1:B:89:PRO:HB3	2.52	0.44
1:C:129:ASN:ND2	1:C:167:GLU:H	2.14	0.44
1:D:50:ASN:ND2	1:D:52:THR:N	2.64	0.44
1:B:130:THR:CG2	1:B:135:MET:CE	2.96	0.44
1:D:50:ASN:ND2	1:D:53:HIS:H	2.15	0.44
1:A:55:ARG:HH12	3:A:202:VK3:H8K1	1.83	0.44
1:C:194:HIS:CE1	4:C:301:HOH:O	2.70	0.44
1:B:153:CYS:O	1:B:154:ALA:HB3	2.19	0.43
1:C:129:ASN:HD21	1:C:167:GLU:H	1.67	0.43
1:C:55:ARG:NH1	3:C:202:VK3:H8K1	2.34	0.43
1:A:164:THR:O	1:A:165:SER:C	2.56	0.43
1:A:170:SER:OG	1:A:173:GLU:HG3	2.18	0.43
1:B:172:ASP:HB2	4:B:346:HOH:O	2.19	0.43
1:A:163:LEU:HB3	1:A:177:LEU:HD13	2.00	0.43
1:B:102:ALA:O	1:B:103:ASP:HB2	2.19	0.43
1:C:145:LEU:O	1:C:150:LEU:HG	2.19	0.43
1:C:129:ASN:HD21	1:C:167:GLU:CG	2.31	0.42
1:D:135:MET:N	1:D:136:PRO:CD	2.82	0.42
1:A:166:ILE:HA	1:A:166:ILE:HD12	1.85	0.42
1:D:115:GLY:O	1:D:118:GLN:OE1	2.38	0.42
1:A:118:GLN:NE2	4:A:398:HOH:O	2.52	0.42
1:C:111:VAL:HG23	4:C:436:HOH:O	2.20	0.42
1:D:140:ASP:OD1	1:D:144:VAL:HB	2.19	0.42
1:D:149:ILE:O	1:D:152:PRO:HD2	2.20	0.42
1:B:47:LEU:HD11	1:B:58:LEU:HD13	2.01	0.42
1:A:156:SER:HA	1:A:157:PRO:C	2.41	0.41
1:B:29:LYS:HD3	1:B:29:LYS:HA	1.72	0.41
3:C:202:VK3:C11	4:C:446:HOH:O	2.69	0.41
4:C:333:HOH:O	3:D:202:VK3:H112	2.20	0.41
1:C:140:ASP:O	1:C:143:LYS:HE2	2.21	0.41
1:D:121:SER:HB3	1:D:157:PRO:HD2	2.02	0.41
1:C:172:ASP:HB3	4:C:379:HOH:O	2.20	0.41
1:A:58:LEU:HA	1:A:61:VAL:HG23	2.03	0.41
1:B:130:THR:HG22	1:B:135:MET:HE3	2.03	0.41
2:A:201:FAD:HM81	1:B:55:ARG:CZ	2.51	0.41
1:B:113:LEU:HD11	3:B:202:VK3:C2K	2.51	0.41
4:C:443:HOH:O	3:D:202:VK3:C8K	2.57	0.41
1:D:166:ILE:O	1:D:174:ARG:HD3	2.21	0.41
1:A:1:MET:HG2	1:A:31:HIS:ND1	2.37	0.40
1:A:55:ARG:NH1	3:A:202:VK3:H8K1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.95	0.40
1:A:11:ASN:HA	1:A:12:PRO:HD3	1.93	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	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
1	B	186/196 (95%)	172 (92%)	14 (8%)	0	100	100
1	C	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
1	D	186/196 (95%)	169 (91%)	16 (9%)	1 (0%)	29	15
All	All	760/784 (97%)	711 (94%)	48 (6%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	111	VAL

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	168/178 (94%)	167 (99%)	1 (1%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	162/178 (91%)	161 (99%)	1 (1%)	86	84
1	C	167/178 (94%)	166 (99%)	1 (1%)	86	84
1	D	158/178 (89%)	151 (96%)	7 (4%)	28	14
All	All	655/712 (92%)	645 (98%)	10 (2%)	65	56

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	THR
1	B	120	LYS
1	C	91	ILE
1	D	34	SER
1	D	50	ASN
1	D	103	ASP
1	D	109	LYS
1	D	118	GLN
1	D	132	SER
1	D	172	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	191	HIS
1	A	192	HIS
1	A	194	HIS
1	A	196	HIS
1	B	24	GLN
1	B	50	ASN
1	B	53	HIS
1	B	175	GLN
1	B	179	HIS
1	C	24	GLN
1	C	116	HIS
1	C	129	ASN
1	C	179	HIS
1	C	183	GLN
1	C	191	HIS
1	C	192	HIS
1	C	194	HIS

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Mol	Chain	Res	Type
1	D	24	GLN
1	D	50	ASN
1	D	118	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	VK3	C	202	-	14,14,14	3.94	7 (50%)	20,20,20	1.21	2 (10%)
2	FAD	D	201	-	51,58,58	5.12	22 (43%)	60,89,89	2.58	18 (30%)
3	VK3	B	202	-	14,14,14	4.08	7 (50%)	20,20,20	1.07	1 (5%)
3	VK3	A	202	-	14,14,14	3.93	7 (50%)	20,20,20	1.35	4 (20%)
2	FAD	B	201	-	51,58,58	5.10	20 (39%)	60,89,89	2.59	20 (33%)
2	FAD	A	201	-	51,58,58	4.96	21 (41%)	60,89,89	2.45	16 (26%)
3	VK3	D	202	-	14,14,14	4.05	8 (57%)	20,20,20	1.14	2 (10%)
2	FAD	C	201	-	51,58,58	4.96	21 (41%)	60,89,89	2.39	16 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VK3	C	202	-	-	-	0/2/2/2
2	FAD	D	201	-	-	5/30/50/50	0/6/6/6
3	VK3	B	202	-	-	-	0/2/2/2
3	VK3	A	202	-	-	-	0/2/2/2
2	FAD	B	201	-	-	3/30/50/50	0/6/6/6
2	FAD	A	201	-	-	3/30/50/50	0/6/6/6
3	VK3	D	202	-	-	-	0/2/2/2
2	FAD	C	201	-	-	0/30/50/50	0/6/6/6

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	FAD	C4X-C10	17.66	1.56	1.38
2	D	201	FAD	C4X-C10	17.44	1.56	1.38
2	C	201	FAD	C4X-C10	16.83	1.55	1.38
2	A	201	FAD	C4X-C10	16.38	1.55	1.38
2	D	201	FAD	C4-N3	15.57	1.60	1.33
2	B	201	FAD	C10-N1	15.40	1.53	1.33
2	C	201	FAD	C4-N3	15.22	1.59	1.33
2	B	201	FAD	C4-N3	15.18	1.59	1.33
2	A	201	FAD	C4-N3	15.11	1.59	1.33
2	D	201	FAD	C10-N1	15.07	1.52	1.33
2	A	201	FAD	C10-N1	14.87	1.52	1.33
2	C	201	FAD	C10-N1	14.21	1.51	1.33
2	D	201	FAD	C4X-N5	9.50	1.46	1.33
2	A	201	FAD	C4X-N5	9.19	1.46	1.33
2	B	201	FAD	C4X-N5	9.13	1.46	1.33
2	C	201	FAD	C4X-N5	9.04	1.46	1.33
2	D	201	FAD	C2-N3	8.92	1.55	1.38
2	B	201	FAD	C2-N3	8.91	1.55	1.38
2	A	201	FAD	C2-N3	8.83	1.55	1.38
2	C	201	FAD	C2-N3	8.59	1.55	1.38
3	C	202	VK3	O4K-C4K	8.57	1.41	1.23
3	B	202	VK3	O4K-C4K	8.56	1.41	1.23
2	D	201	FAD	C4-C4X	8.51	1.56	1.41
2	B	201	FAD	C4-C4X	8.45	1.55	1.41
3	D	202	VK3	O4K-C4K	8.44	1.41	1.23
3	A	202	VK3	O4K-C4K	8.35	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	FAD	C2-N1	8.11	1.54	1.38
2	A	201	FAD	C2-N1	8.02	1.54	1.38
2	C	201	FAD	C4-C4X	8.00	1.55	1.41
2	C	201	FAD	C2-N1	7.96	1.53	1.38
2	D	201	FAD	C2-N1	7.91	1.53	1.38
2	A	201	FAD	C4-C4X	7.89	1.54	1.41
3	D	202	VK3	O1K-C1K	7.66	1.41	1.24
3	B	202	VK3	O1K-C1K	7.42	1.40	1.24
3	C	202	VK3	O1K-C1K	7.03	1.39	1.24
3	A	202	VK3	O1K-C1K	7.02	1.39	1.24
3	B	202	VK3	C10-C1K	-6.82	1.36	1.48
2	D	201	FAD	C5X-N5	6.66	1.46	1.35
3	A	202	VK3	C10-C1K	-6.62	1.36	1.48
3	D	202	VK3	C10-C1K	-6.56	1.36	1.48
2	D	201	FAD	O4-C4	6.44	1.40	1.24
2	B	201	FAD	O4-C4	6.33	1.40	1.24
2	B	201	FAD	C5X-N5	6.31	1.45	1.35
3	C	202	VK3	C10-C1K	-6.30	1.37	1.48
2	C	201	FAD	C5X-N5	6.28	1.45	1.35
2	A	201	FAD	C5X-N5	6.13	1.45	1.35
2	B	201	FAD	C9A-C5X	-5.90	1.30	1.42
2	C	201	FAD	O4-C4	5.88	1.39	1.24
2	A	201	FAD	O4-C4	5.87	1.39	1.24
2	C	201	FAD	C9A-C5X	-5.70	1.31	1.42
2	A	201	FAD	C9A-C5X	-5.66	1.31	1.42
2	D	201	FAD	C9A-C5X	-5.58	1.31	1.42
2	A	201	FAD	C9A-N10	4.80	1.45	1.38
2	B	201	FAD	C9A-N10	4.45	1.44	1.38
2	D	201	FAD	C9A-N10	4.43	1.44	1.38
2	C	201	FAD	C9A-N10	4.33	1.44	1.38
3	B	202	VK3	C8K-C7K	4.25	1.49	1.38
3	A	202	VK3	C8K-C7K	4.18	1.49	1.38
2	C	201	FAD	PA-O1A	4.13	1.65	1.50
3	C	202	VK3	C8K-C7K	4.10	1.48	1.38
3	D	202	VK3	C8K-C7K	4.09	1.48	1.38
3	C	202	VK3	C3K-C4K	-4.03	1.42	1.48
2	A	201	FAD	P-O1P	3.98	1.65	1.50
3	B	202	VK3	C3K-C4K	-3.98	1.42	1.48
2	A	201	FAD	PA-O1A	3.97	1.65	1.50
2	C	201	FAD	P-O1P	3.96	1.65	1.50
3	A	202	VK3	C3K-C4K	-3.93	1.42	1.48
2	B	201	FAD	PA-O1A	3.92	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	FAD	PA-O1A	3.91	1.64	1.50
2	D	201	FAD	P-O1P	3.89	1.64	1.50
2	C	201	FAD	C2B-C1B	-3.87	1.47	1.53
3	D	202	VK3	C3K-C4K	-3.75	1.42	1.48
2	B	201	FAD	P-O1P	3.72	1.64	1.50
2	A	201	FAD	C2B-C1B	-3.65	1.48	1.53
2	D	201	FAD	C2B-C1B	-3.41	1.48	1.53
2	D	201	FAD	C1'-N10	-3.39	1.44	1.48
2	C	201	FAD	C1'-N10	-3.39	1.44	1.48
2	B	201	FAD	C2B-C1B	-3.37	1.48	1.53
2	A	201	FAD	C6A-N6A	3.26	1.45	1.34
2	D	201	FAD	C6A-N6A	3.25	1.45	1.34
2	C	201	FAD	C6A-N6A	3.19	1.45	1.34
2	B	201	FAD	C6A-N6A	3.11	1.45	1.34
2	A	201	FAD	C1'-N10	-2.96	1.45	1.48
2	B	201	FAD	C1'-N10	-2.96	1.45	1.48
2	A	201	FAD	C2A-N3A	2.77	1.36	1.32
2	C	201	FAD	C2A-N3A	2.58	1.36	1.32
3	C	202	VK3	C5K-C4K	-2.55	1.43	1.48
2	C	201	FAD	C3B-C4B	2.55	1.59	1.53
3	D	202	VK3	C5K-C4K	-2.52	1.43	1.48
2	C	201	FAD	C8A-N7A	2.52	1.39	1.34
2	D	201	FAD	C5A-C4A	-2.48	1.34	1.40
3	B	202	VK3	C10-C5K	2.43	1.44	1.40
3	D	202	VK3	C10-C5K	2.38	1.44	1.40
2	B	201	FAD	C8A-N7A	2.37	1.38	1.34
2	D	201	FAD	C8A-N7A	2.35	1.38	1.34
2	A	201	FAD	C5A-C4A	-2.35	1.34	1.40
2	A	201	FAD	C8A-N7A	2.34	1.38	1.34
2	D	201	FAD	C2A-N3A	2.33	1.35	1.32
3	A	202	VK3	C10-C5K	2.32	1.44	1.40
2	B	201	FAD	C2A-N3A	2.31	1.35	1.32
3	B	202	VK3	C2K-C1K	2.26	1.49	1.44
2	B	201	FAD	C5A-C4A	-2.25	1.35	1.40
2	A	201	FAD	C3B-C4B	2.25	1.58	1.53
3	A	202	VK3	C5K-C4K	-2.24	1.43	1.48
2	D	201	FAD	C3B-C4B	2.22	1.58	1.53
3	D	202	VK3	C2K-C1K	2.22	1.49	1.44
2	C	201	FAD	C5A-C4A	-2.20	1.35	1.40
3	C	202	VK3	C10-C5K	2.18	1.44	1.40
2	D	201	FAD	C8-C7	-2.17	1.35	1.40
2	B	201	FAD	C3B-C4B	2.13	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	FAD	C8-C7	-2.10	1.35	1.40
2	C	201	FAD	C8-C7	-2.05	1.35	1.40
2	D	201	FAD	PA-O2A	-2.01	1.45	1.55

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	FAD	C10-C4X-N5	-9.92	114.40	121.26
2	D	201	FAD	C10-C4X-N5	-9.76	114.51	121.26
2	B	201	FAD	C4X-C4-N3	-8.34	112.02	123.43
2	C	201	FAD	C4X-C4-N3	-8.20	112.22	123.43
2	C	201	FAD	C10-C4X-N5	-7.95	115.76	121.26
2	A	201	FAD	C4-N3-C2	7.43	121.41	115.14
2	D	201	FAD	C4X-C4-N3	-7.32	113.42	123.43
2	D	201	FAD	C4-N3-C2	7.30	121.31	115.14
2	A	201	FAD	C4X-C4-N3	-7.16	113.64	123.43
2	A	201	FAD	C10-C4X-N5	-6.76	116.58	121.26
2	A	201	FAD	C5X-C9A-N10	6.00	122.06	117.72
2	A	201	FAD	N3A-C2A-N1A	-5.97	119.35	128.68
2	D	201	FAD	N3A-C2A-N1A	-5.68	119.79	128.68
2	B	201	FAD	N3A-C2A-N1A	-5.66	119.83	128.68
2	D	201	FAD	C4X-N5-C5X	5.66	122.42	116.77
2	C	201	FAD	N3A-C2A-N1A	-5.55	120.00	128.68
2	C	201	FAD	C5X-C9A-N10	5.29	121.55	117.72
2	B	201	FAD	C4-N3-C2	5.00	119.36	115.14
2	A	201	FAD	C4X-N5-C5X	4.92	121.69	116.77
2	B	201	FAD	C5X-C9A-N10	4.82	121.21	117.72
2	D	201	FAD	C5X-C9A-N10	4.60	121.05	117.72
2	A	201	FAD	C4X-C10-N10	-4.57	115.60	120.30
2	C	201	FAD	C4X-C10-N10	-4.54	115.64	120.30
2	B	201	FAD	C4X-N5-C5X	4.46	121.23	116.77
2	C	201	FAD	C4X-N5-C5X	3.84	120.61	116.77
2	C	201	FAD	C4-C4X-N5	3.81	122.96	118.60
2	B	201	FAD	C4X-C10-N10	-3.73	116.47	120.30
2	C	201	FAD	O3B-C3B-C4B	3.33	120.68	111.05
2	D	201	FAD	C4X-C10-N10	-3.19	117.02	120.30
2	C	201	FAD	C1'-N10-C9A	3.04	120.69	118.29
3	A	202	VK3	C11-C3K-C4K	3.03	121.24	117.72
2	B	201	FAD	O2B-C2B-C1B	2.98	121.86	110.85
2	B	201	FAD	O3B-C3B-C2B	2.94	121.34	111.82
3	C	202	VK3	C3K-C2K-C1K	-2.90	119.33	123.27
2	B	201	FAD	O3'-C3'-C4'	2.88	115.77	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	FAD	O3B-C3B-C4B	2.87	119.34	111.05
2	D	201	FAD	O3B-C3B-C4B	2.81	119.19	111.05
2	D	201	FAD	C4-C4X-C10	-2.79	118.10	119.95
2	B	201	FAD	O4'-C4'-C3'	2.79	115.87	109.10
3	A	202	VK3	C3K-C2K-C1K	-2.78	119.49	123.27
2	D	201	FAD	O2B-C2B-C1B	2.78	121.10	110.85
2	B	201	FAD	C1'-N10-C9A	2.76	120.47	118.29
2	C	201	FAD	O3B-C3B-C2B	2.76	120.75	111.82
2	D	201	FAD	O3'-C3'-C4'	2.74	115.42	108.81
2	A	201	FAD	C4-C4X-N5	2.71	121.70	118.60
2	B	201	FAD	C1B-N9A-C4A	-2.70	121.89	126.64
2	A	201	FAD	O2'-C2'-C1'	2.68	116.06	109.59
3	D	202	VK3	C11-C3K-C4K	2.66	120.81	117.72
2	C	201	FAD	O2'-C2'-C3'	2.66	115.57	109.10
2	C	201	FAD	O2B-C2B-C3B	2.56	120.10	111.82
2	D	201	FAD	O4'-C4'-C3'	2.54	115.28	109.10
3	D	202	VK3	C3K-C2K-C1K	-2.53	119.83	123.27
2	B	201	FAD	O2'-C2'-C1'	2.50	115.61	109.59
2	B	201	FAD	C6-C5X-N5	-2.48	116.31	119.05
2	D	201	FAD	O4B-C1B-C2B	2.47	110.54	106.93
2	B	201	FAD	O3B-C3B-C4B	2.46	118.15	111.05
2	B	201	FAD	O2B-C2B-C3B	2.44	119.70	111.82
3	B	202	VK3	C3K-C2K-C1K	-2.43	119.97	123.27
2	A	201	FAD	O2B-C2B-C1B	2.42	119.79	110.85
2	B	201	FAD	C4-C4X-N5	2.36	121.29	118.60
2	C	201	FAD	O2B-C2B-C1B	2.33	119.46	110.85
3	C	202	VK3	O1K-C1K-C2K	-2.31	117.93	121.79
2	D	201	FAD	O2'-C2'-C3'	2.30	114.70	109.10
2	D	201	FAD	C1'-N10-C9A	2.28	120.08	118.29
2	D	201	FAD	O3B-C3B-C2B	2.27	119.15	111.82
2	B	201	FAD	C4-C4X-C10	-2.24	118.47	119.95
2	C	201	FAD	O5'-C5'-C4'	2.24	115.33	109.36
2	A	201	FAD	O3B-C3B-C2B	2.23	119.04	111.82
2	C	201	FAD	O2'-C2'-C1'	2.21	114.91	109.59
2	A	201	FAD	C1'-N10-C9A	2.21	120.03	118.29
3	A	202	VK3	O1K-C1K-C2K	-2.19	118.14	121.79
3	A	202	VK3	C10-C1K-C2K	2.18	121.08	116.63
2	A	201	FAD	O4'-C4'-C3'	2.17	114.37	109.10
2	D	201	FAD	C4-C4X-N5	2.17	121.08	118.60
2	A	201	FAD	O4B-C4B-C5B	2.12	116.34	109.37
2	A	201	FAD	O2'-C2'-C3'	2.06	114.12	109.10
2	D	201	FAD	O2B-C2B-C3B	2.06	118.48	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	FAD	O4B-C1B-C2B	2.02	109.89	106.93
2	B	201	FAD	C1'-N10-C10	-2.01	116.61	118.41

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	FAD	C3'-C4'-C5'-O5'
2	D	201	FAD	P-O3P-PA-O1A
2	A	201	FAD	C4'-C5'-O5'-P
2	D	201	FAD	C5'-O5'-P-O3P
2	D	201	FAD	C4'-C5'-O5'-P
2	B	201	FAD	C4'-C5'-O5'-P
2	A	201	FAD	P-O3P-PA-O2A
2	D	201	FAD	P-O3P-PA-O2A
2	D	201	FAD	C3'-C4'-C5'-O5'
2	B	201	FAD	C5B-O5B-PA-O1A
2	A	201	FAD	C5B-O5B-PA-O1A

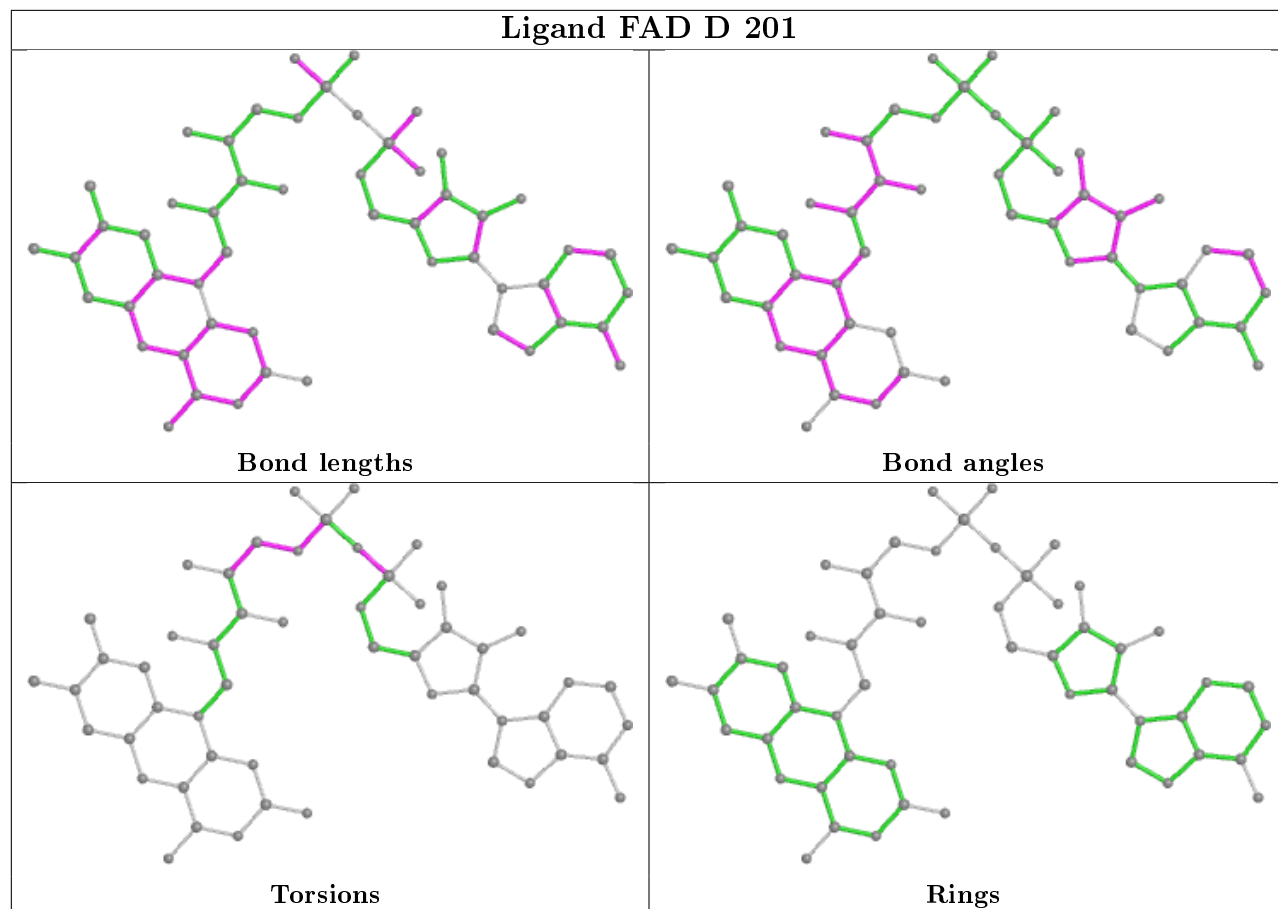
There are no ring outliers.

7 monomers are involved in 24 short contacts:

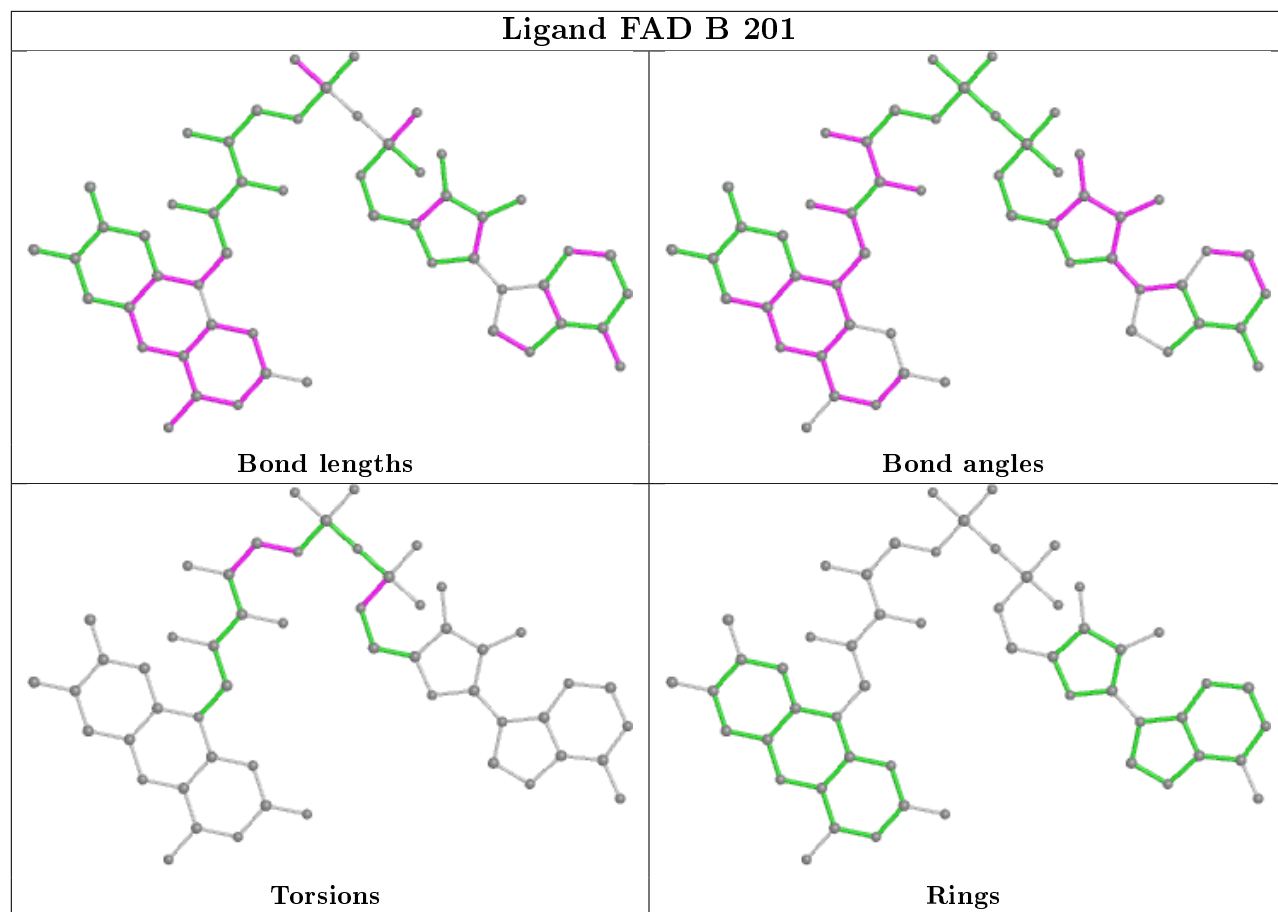
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	202	VK3	6	0
3	B	202	VK3	4	0
3	A	202	VK3	4	0
2	B	201	FAD	1	0
2	A	201	FAD	3	0
3	D	202	VK3	5	0
2	C	201	FAD	1	0

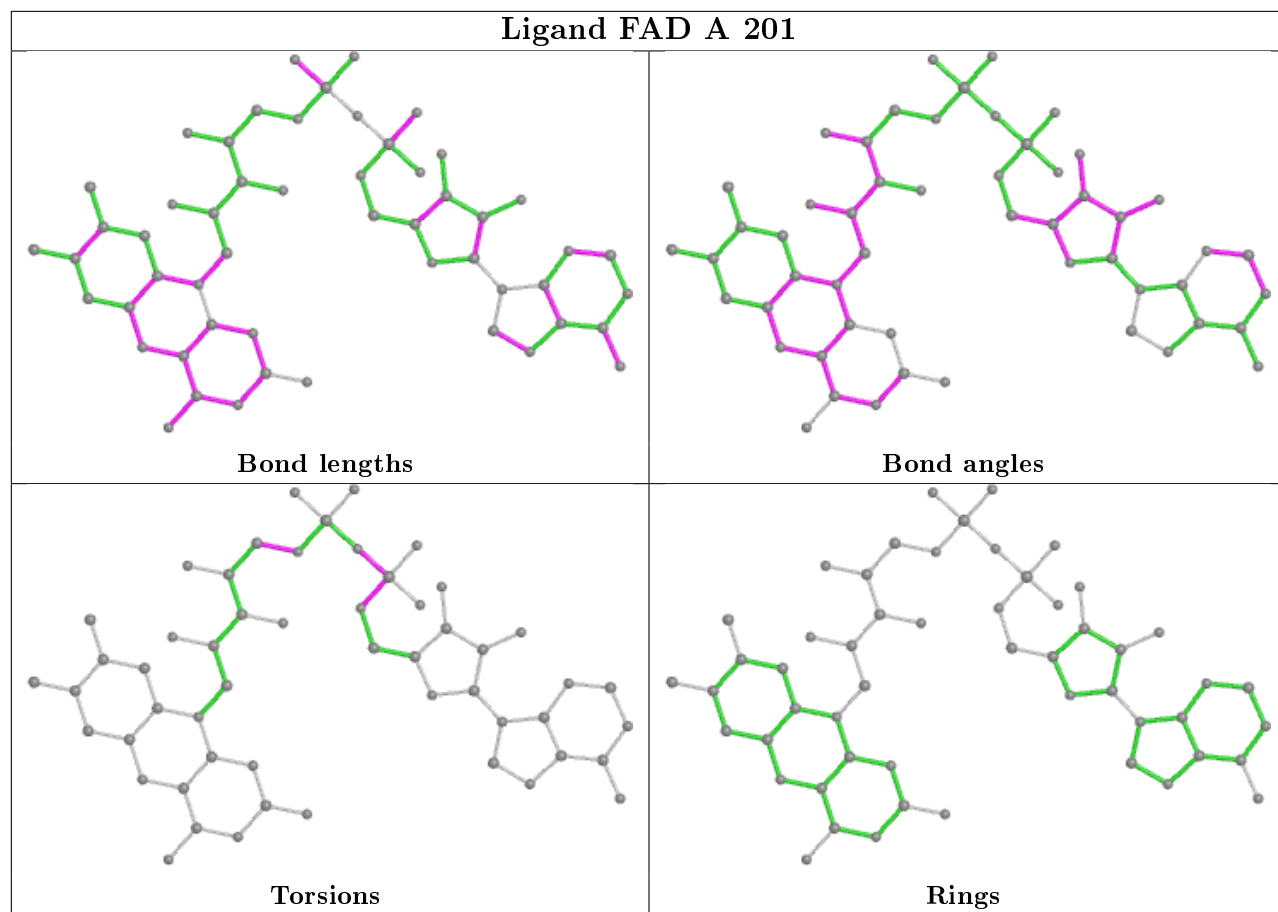
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

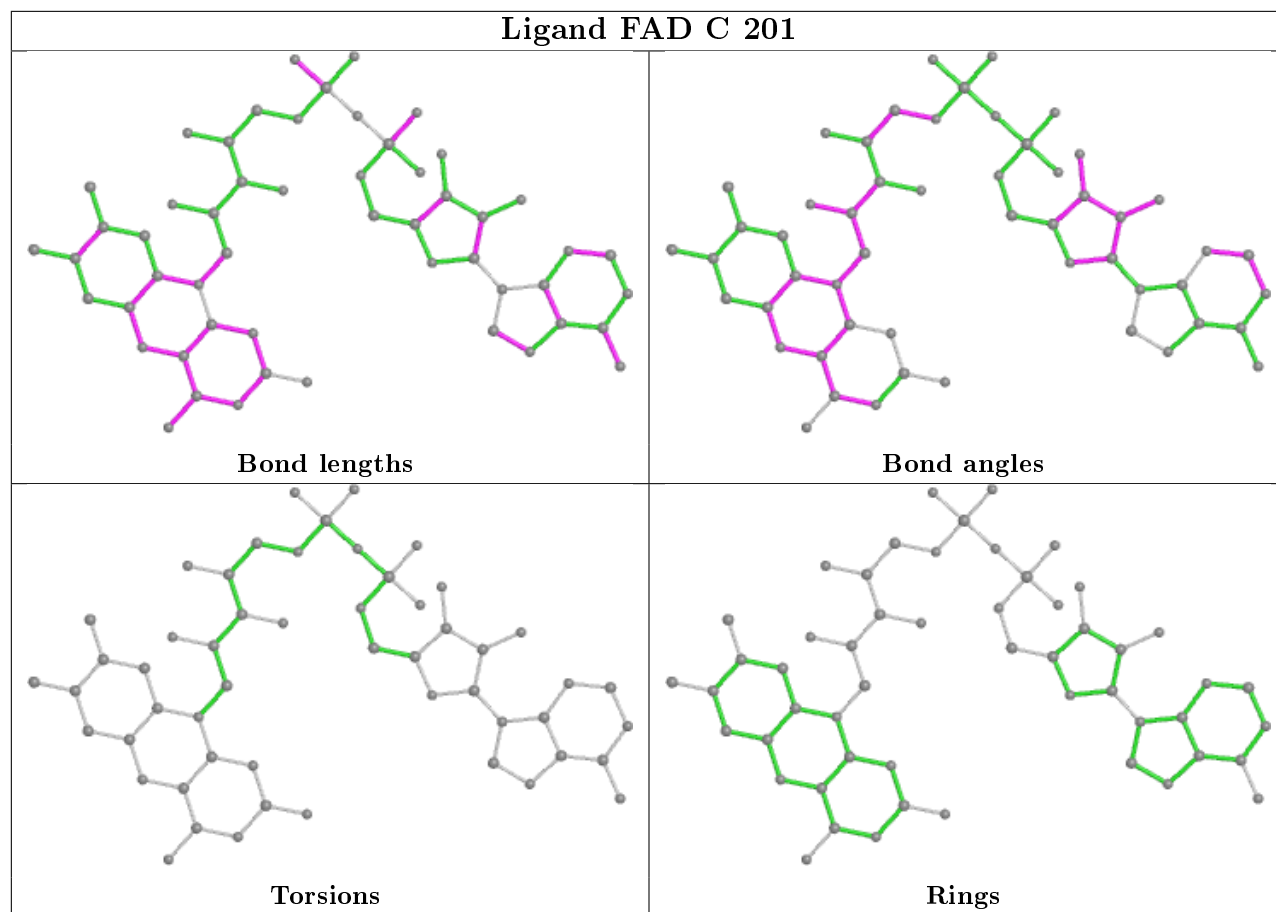
equivalents in the CSD to analyse the geometry.



Ligand FAD B 201







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	196/196 (100%)	-0.58	0 100 100	11, 16, 27, 42	0
1	B	188/196 (95%)	-0.53	0 100 100	11, 17, 29, 49	0
1	C	196/196 (100%)	-0.56	0 100 100	12, 18, 28, 36	0
1	D	188/196 (95%)	-0.50	0 100 100	13, 20, 28, 44	0
All	All	768/784 (97%)	-0.54	0 100 100	11, 17, 28, 49	0

There are no RSRZ outliers to report.

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 carbohydrates 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, 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
3	VK3	D	202	13/13	0.88	0.14	19,22,25,26	0
3	VK3	B	202	13/13	0.89	0.17	22,24,28,32	0
3	VK3	A	202	13/13	0.90	0.15	16,21,24,29	0
3	VK3	C	202	13/13	0.90	0.16	19,24,28,28	0

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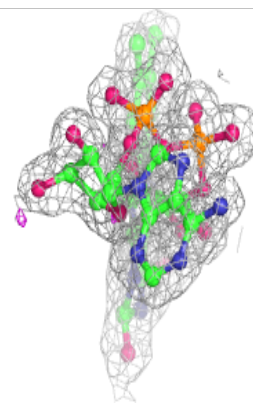
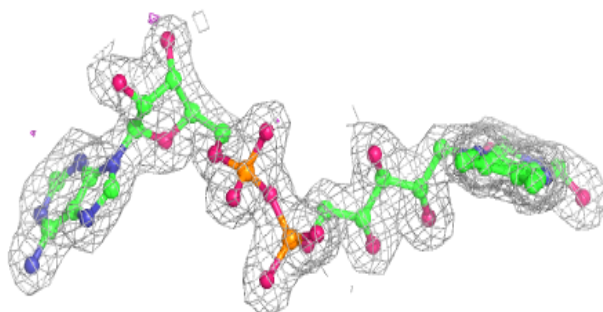
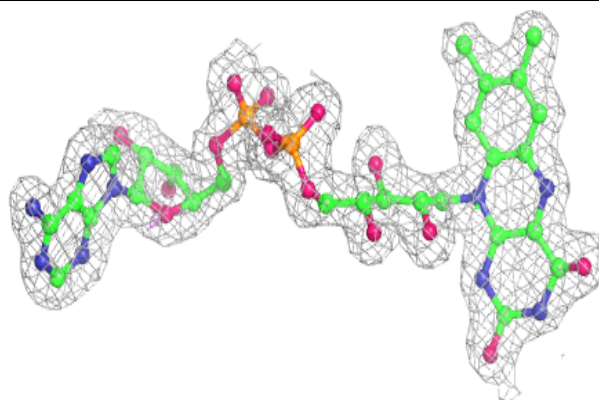
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	A	201	53/53	0.97	0.08	13,18,24,29	0
2	FAD	D	201	53/53	0.97	0.08	15,20,23,25	0
2	FAD	B	201	53/53	0.98	0.07	12,15,18,20	0
2	FAD	C	201	53/53	0.98	0.07	14,18,26,28	0

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.

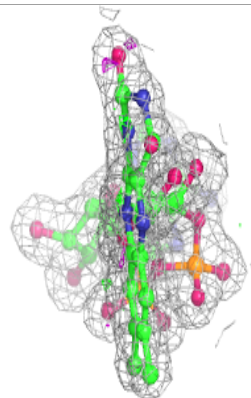
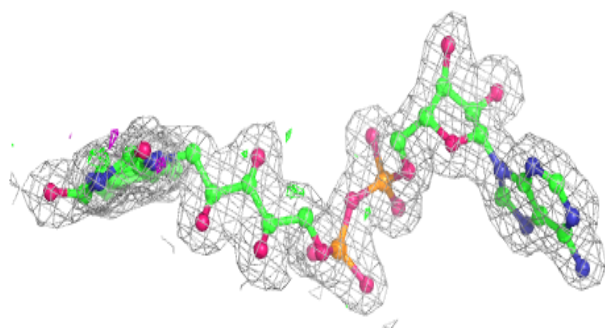
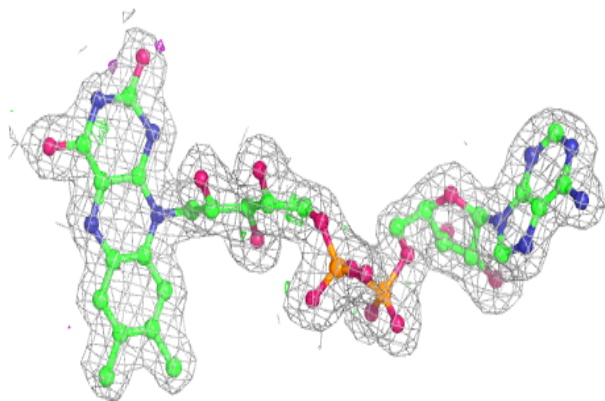
Electron density around FAD A 201:

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

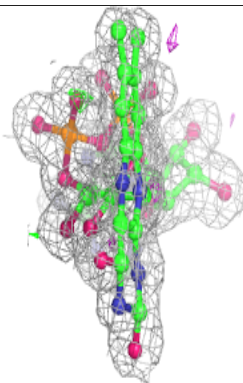
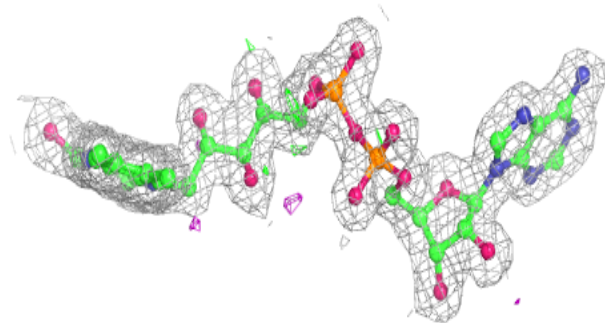
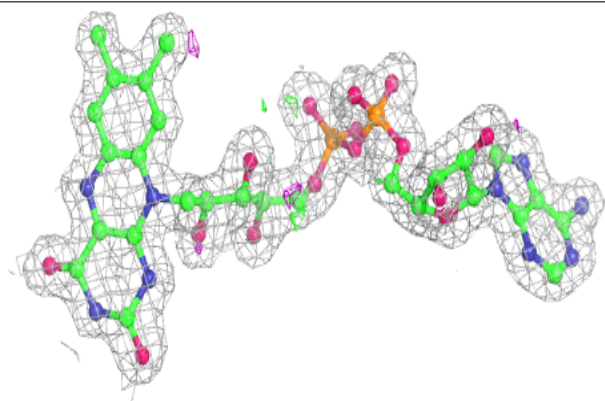


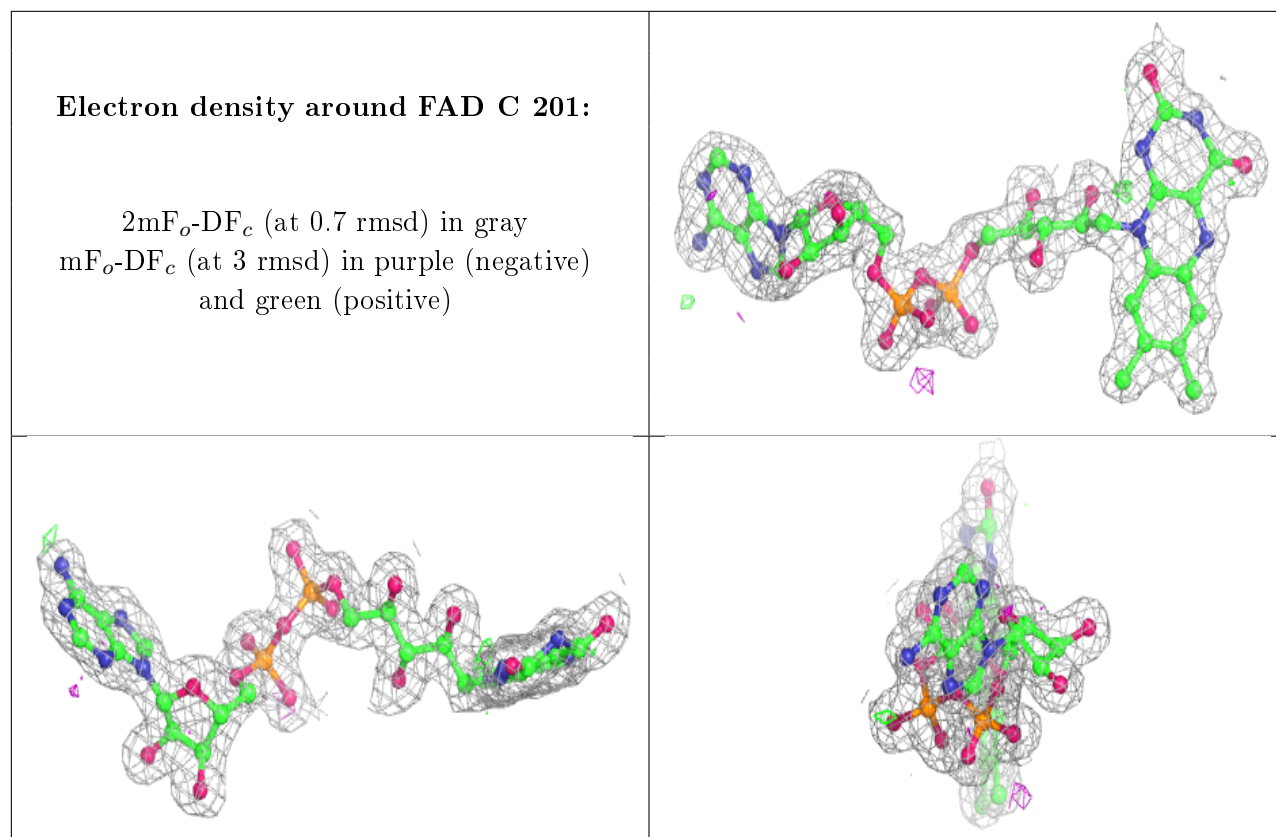
Electron density around FAD D 201:

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

**Electron density around FAD B 201:**

$2mF_o-DF_c$ (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.