



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 03:48 AM EDT

PDB ID : 5URD
Title : wild type rat CYPOR bound with NADP⁺ - oxidized form
Authors : Xia, C.; Kim, J.J.
Deposited on : 2017-02-10
Resolution : 1.90 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

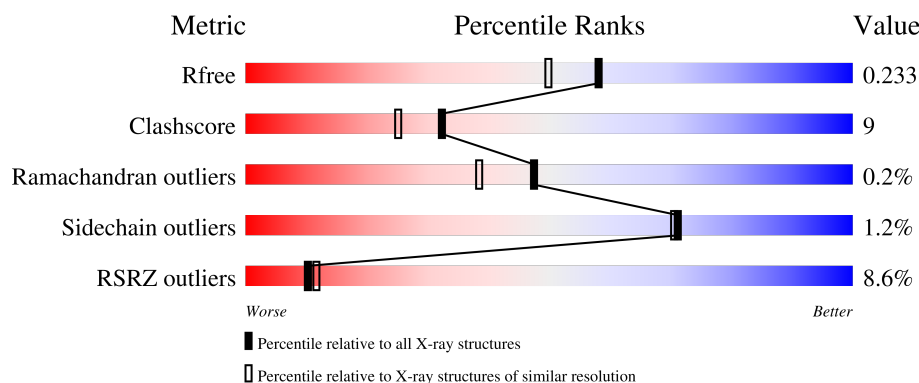
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	622	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	B	622	<div> <div>15%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10640 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-cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4870	3088	835	924	23			
1	B	605	Total	C	N	O	S	0	0	0
			4804	3044	829	908	23			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



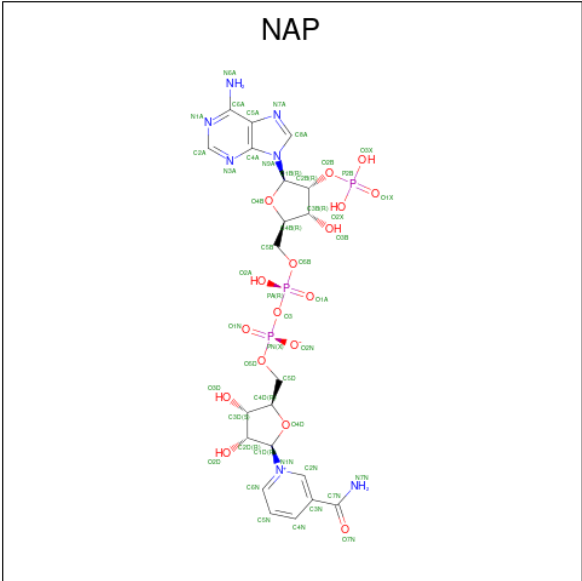
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			34	13	5	13	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

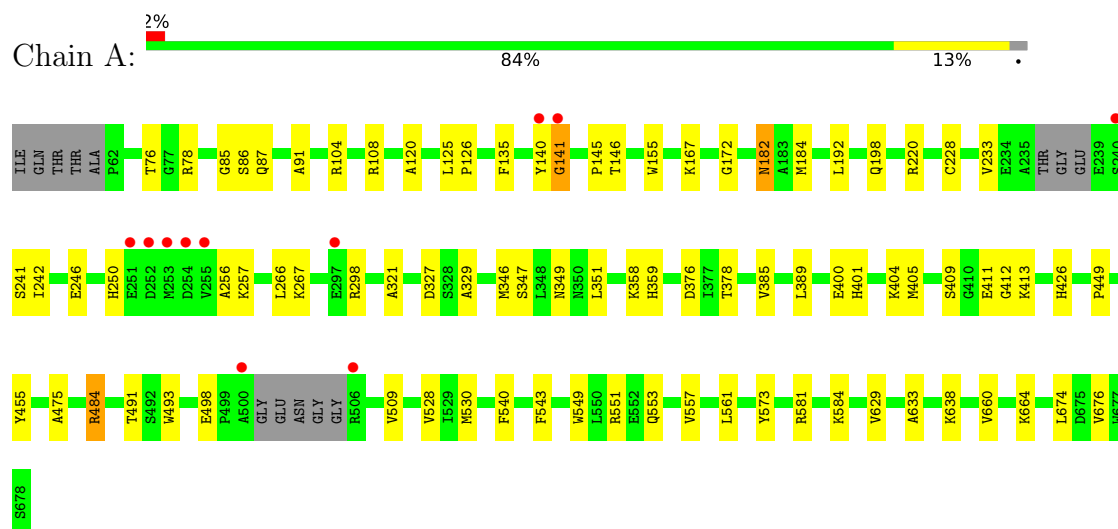
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	399	Total	O	0	0
			399	399		
6	B	324	Total	O	0	0
			324	324		

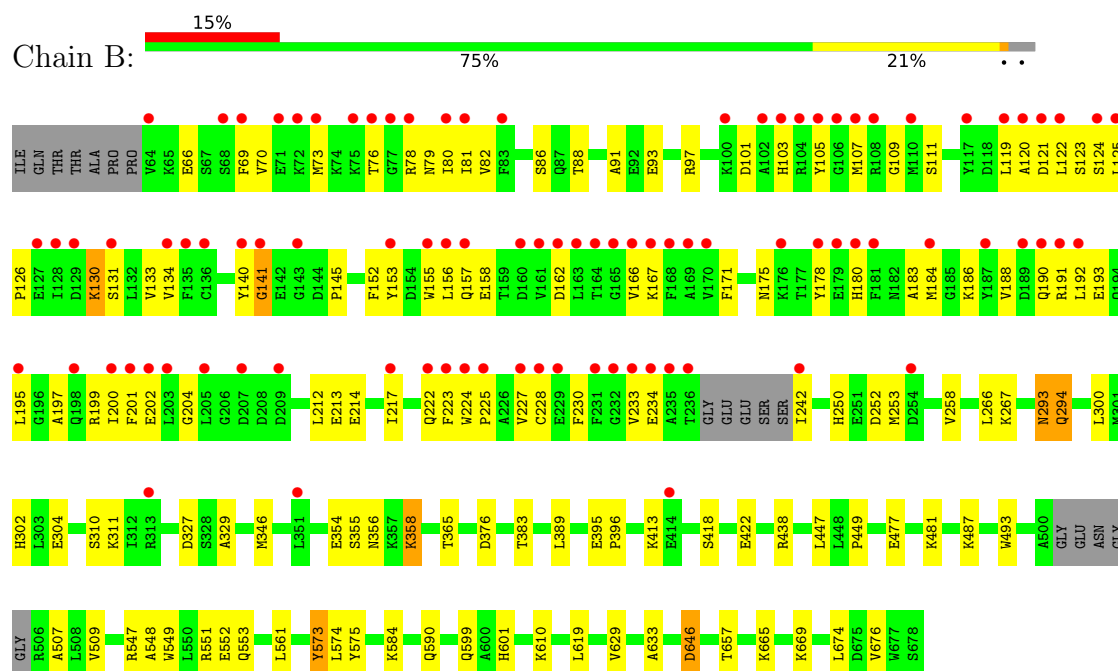
3 Residue-property plots [i](#)

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: NADPH-cytochrome P450 reductase



• Molecule 1: NADPH-cytochrome P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.18Å 114.93Å 117.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 1.90 49.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.97-1.90) 97.4 (49.97-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 1.91Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.205 , 0.239 0.200 , 0.233	Depositor DCC
R_{free} test set	5293 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10640	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.33% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, FAD, PO4, FMN

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	0/4987	0.58	1/6750 (0.0%)
1	B	0.33	0/4919	0.60	4/6660 (0.1%)
All	All	0.33	0/9906	0.59	5/13410 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	507	ALA	N-CA-CB	7.34	120.38	110.10
1	B	130	LYS	N-CA-CB	6.52	122.33	110.60
1	B	158	GLU	N-CA-C	5.98	127.15	111.00
1	A	85	GLY	N-CA-C	-5.60	99.10	113.10
1	B	158	GLU	CB-CA-C	-5.24	99.93	110.40

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	4870	0	4709	52	0
1	B	4804	0	4594	119	0
2	A	31	0	19	0	0
2	B	31	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	31	0	11	0	0
4	B	34	0	13	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	399	0	0	6	0
6	B	324	0	0	6	0
All	All	10640	0	9427	171	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 9.

All (171) 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:228:CYS:CB	1:B:233:VAL:O	2.11	0.98
1:B:228:CYS:HB3	1:B:233:VAL:O	1.73	0.88
1:B:228:CYS:CA	1:B:233:VAL:O	2.22	0.88
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.56	0.85
1:B:228:CYS:HA	1:B:233:VAL:O	1.78	0.83
1:B:293:ASN:H	1:B:293:ASN:HD22	1.26	0.83
1:B:355:SER:O	1:B:358:LYS:HE2	1.78	0.82
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.64	0.78
1:B:358:LYS:N	1:B:358:LYS:HD2	2.01	0.75
1:B:145:PRO:HB3	1:B:184:MET:SD	2.27	0.75
1:B:250:HIS:HB3	1:B:253:MET:HG2	1.73	0.69
1:B:549:TRP:O	1:B:553:GLN:HG2	1.93	0.68
1:B:140:TYR:O	1:B:141:GLY:O	2.12	0.68
1:B:217:ILE:HD11	1:B:383:THR:HG21	1.76	0.68
1:B:228:CYS:HB3	1:B:234:GLU:HA	1.76	0.67
1:B:125:LEU:HD23	1:B:166:VAL:HG13	1.77	0.66
1:A:581:ARG:NH2	1:A:584:LYS:HD3	2.11	0.65
1:B:477:GLU:HG3	1:B:487:LYS:HD2	1.77	0.65
1:B:119:LEU:HG	1:B:152:PHE:CD1	2.32	0.65
1:A:660:VAL:O	1:A:664:LYS:HG2	1.95	0.65
1:B:294:GLN:NE2	1:B:294:GLN:H	1.96	0.64
1:B:302:HIS:HD2	1:B:575:TYR:OH	1.81	0.64
1:B:665:LYS:HE2	1:B:669:LYS:HE3	1.81	0.62
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.80	0.62
1:B:175:ASN:HB3	1:B:178:TYR:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:O	1:B:227:VAL:HG23	2.00	0.61
1:B:120:ALA:HA	1:B:155:TRP:CZ2	2.36	0.61
1:B:66:GLU:HG3	1:B:356:ASN:OD1	2.00	0.60
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.83	0.59
1:B:657:THR:HG23	6:B:1012:HOH:O	2.02	0.59
1:B:140:TYR:CE1	2:B:701:FMN:H5'2	2.37	0.59
1:B:258:VAL:HG13	1:B:365:THR:HA	1.83	0.59
1:B:202:GLU:HB2	6:B:890:HOH:O	2.02	0.58
1:A:256:ALA:HA	1:A:267:LYS:NZ	2.18	0.58
1:B:80:ILE:O	1:B:109:GLY:HA2	2.02	0.58
1:B:252:ASP:O	1:B:252:ASP:OD1	2.20	0.58
1:B:82:VAL:HG22	1:B:134:VAL:HB	1.85	0.58
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.86	0.57
1:B:629:VAL:HB	1:B:674:LEU:HD23	1.85	0.57
1:A:78:ARG:HE	1:A:108:ARG:HG2	1.70	0.56
1:B:153:TYR:O	1:B:157:GLN:HG2	2.05	0.56
1:B:167:LYS:N	1:B:167:LYS:HD2	2.20	0.56
1:B:70:VAL:HG11	1:B:124:SER:O	2.05	0.56
1:B:665:LYS:HE2	1:B:669:LYS:NZ	2.20	0.56
1:B:610:LYS:NZ	1:B:646:ASP:HB3	2.20	0.56
1:B:188:VAL:O	1:B:192:LEU:HG	2.05	0.56
1:A:104:ARG:HH22	1:A:220:ARG:NH2	2.03	0.55
1:A:145:PRO:HB3	1:A:184:MET:SD	2.45	0.55
1:B:69:PHE:CE1	1:B:121:ASP:HB2	2.41	0.55
1:B:73:MET:HB3	1:B:78:ARG:O	2.05	0.55
1:B:140:TYR:O	1:B:141:GLY:C	2.45	0.55
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.89	0.55
1:B:665:LYS:HE2	1:B:669:LYS:CE	2.36	0.55
1:B:186:LYS:O	1:B:190:GLN:HG2	2.07	0.54
1:A:241:SER:C	1:A:242:ILE:HD12	2.28	0.54
1:B:79:ASN:O	1:B:131:SER:HA	2.08	0.53
1:B:599:GLN:HG3	1:B:601:HIS:CE1	2.44	0.53
1:B:230:PHE:HB2	6:B:841:HOH:O	2.07	0.53
1:A:242:ILE:HD12	1:A:242:ILE:N	2.24	0.53
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.91	0.53
1:B:481:LYS:HE3	6:B:896:HOH:O	2.09	0.52
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.90	0.52
1:A:87:GLN:HB3	1:A:140:TYR:CZ	2.44	0.52
1:B:300:LEU:HD22	1:B:574:LEU:HD21	1.91	0.52
1:B:293:ASN:HD22	1:B:293:ASN:N	1.98	0.52
1:A:141:GLY:HA2	6:A:830:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.93	0.51
1:B:294:GLN:HE22	1:B:573:TYR:H	1.60	0.50
1:B:548:ALA:O	1:B:552:GLU:HG2	2.12	0.50
1:A:172:GLY:C	1:A:182:ASN:HD21	2.15	0.49
1:B:70:VAL:HA	1:B:73:MET:HE3	1.94	0.49
1:B:294:GLN:H	1:B:294:GLN:HE21	1.60	0.49
1:B:167:LYS:CG	1:B:200:ILE:HD11	2.43	0.49
1:B:547:ARG:O	1:B:551:ARG:HG3	2.13	0.49
1:A:561:LEU:HD12	1:A:561:LEU:N	2.27	0.49
1:A:498:GLU:HG2	6:A:1098:HOH:O	2.13	0.49
1:B:152:PHE:CZ	1:B:156:LEU:HD11	2.48	0.49
1:B:73:MET:CB	1:B:78:ARG:HB2	2.43	0.49
1:B:81:ILE:HG23	1:B:81:ILE:O	2.12	0.49
1:A:228:CYS:HA	1:A:233:VAL:CG2	2.43	0.48
1:B:302:HIS:HE1	1:B:304:GLU:OE1	1.96	0.48
1:B:201:PHE:HZ	1:B:222:GLN:HB2	1.77	0.48
1:B:190:GLN:HG3	1:B:191:ARG:N	2.28	0.48
1:B:222:GLN:C	1:B:225:PRO:HD2	2.34	0.48
1:A:120:ALA:HA	1:A:155:TRP:CZ2	2.49	0.48
1:B:180:HIS:HB3	1:B:183:ALA:HB2	1.96	0.48
1:B:125:LEU:N	1:B:126:PRO:CD	2.77	0.47
1:B:191:ARG:O	1:B:195:LEU:HD13	2.14	0.47
1:B:105:TYR:O	1:B:107:MET:HG3	2.14	0.47
1:B:119:LEU:HD22	1:B:119:LEU:N	2.30	0.47
1:A:638:LYS:HB2	6:A:802:HOH:O	2.13	0.47
1:B:665:LYS:HD3	6:B:968:HOH:O	2.14	0.47
1:B:70:VAL:HA	1:B:73:MET:CE	2.44	0.47
1:B:70:VAL:HG21	1:B:121:ASP:O	2.15	0.47
1:B:193:GLU:HA	1:B:197:ALA:O	2.14	0.47
1:B:214:GLU:OE1	1:B:413:LYS:HE3	2.15	0.47
1:B:79:ASN:HD21	1:B:107:MET:CG	2.28	0.47
1:B:101:ASP:HB2	1:B:224:TRP:CZ2	2.50	0.47
1:B:167:LYS:HB3	1:B:200:ILE:CG1	2.45	0.47
1:B:73:MET:HA	1:B:78:ARG:HB2	1.96	0.47
1:B:584:LYS:O	1:B:584:LYS:HD3	2.15	0.47
1:A:327:ASP:OD1	1:A:329:ALA:HB3	2.15	0.46
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.80	0.46
1:B:82:VAL:O	1:B:111:SER:HA	2.15	0.46
1:B:79:ASN:HB2	1:B:130:LYS:O	2.15	0.46
1:B:73:MET:CA	1:B:78:ARG:HB2	2.46	0.46
1:B:493:TRP:CH2	1:B:509:VAL:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ALA:HA	1:A:267:LYS:HZ1	1.80	0.46
1:B:438:ARG:HH21	1:B:438:ARG:HG2	1.80	0.45
1:A:167:LYS:HE3	1:A:198:GLN:OE1	2.16	0.45
1:A:321:ALA:HB2	1:A:455:TYR:CE1	2.51	0.45
1:A:528:VAL:HG12	1:A:530:MET:HG3	1.98	0.45
1:B:133:VAL:O	1:B:133:VAL:HG13	2.15	0.45
1:B:228:CYS:SG	1:B:233:VAL:O	2.74	0.45
1:A:409:SER:HA	1:A:413:LYS:HD3	1.99	0.45
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.99	0.45
1:B:140:TYR:HE1	2:B:701:FMN:H5'2	1.81	0.45
1:B:266:LEU:O	1:B:267:LYS:HB2	2.16	0.45
1:A:298:ARG:HD3	6:A:872:HOH:O	2.16	0.45
1:B:93:GLU:O	1:B:97:ARG:HG3	2.17	0.45
1:A:135:PHE:CE2	1:A:192:LEU:HD11	2.52	0.44
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.99	0.44
1:B:88:THR:HG22	6:B:1080:HOH:O	2.16	0.44
1:B:103:HIS:CG	1:B:242:ILE:HD12	2.52	0.44
1:B:358:LYS:HD2	1:B:358:LYS:H	1.79	0.44
1:A:549:TRP:O	1:A:553:GLN:HG2	2.17	0.44
1:B:76:THR:HG21	1:B:354:GLU:HG2	1.99	0.44
1:A:385:VAL:O	1:A:389:LEU:HG	2.17	0.43
1:B:123:SER:O	1:B:126:PRO:HD2	2.18	0.43
1:B:389:LEU:HD21	1:B:447:LEU:HD12	2.00	0.43
1:B:418:SER:HA	1:B:422:GLU:HB3	1.99	0.43
1:B:103:HIS:HA	1:B:107:MET:O	2.18	0.43
1:B:310:SER:O	1:B:311:LYS:HB2	2.18	0.43
1:A:250:HIS:HE1	1:A:347:SER:OG	2.00	0.43
1:B:633:ALA:HB2	1:B:676:VAL:HB	2.00	0.43
1:B:175:ASN:HB3	1:B:178:TYR:CD2	2.50	0.43
1:B:213:GLU:O	1:B:217:ILE:HG13	2.18	0.43
1:A:267:LYS:HA	6:A:1094:HOH:O	2.17	0.43
1:B:422:GLU:HG3	1:B:481:LYS:HE2	2.00	0.43
1:A:76:THR:OG1	1:A:78:ARG:HD3	2.19	0.43
1:A:256:ALA:HA	1:A:267:LYS:HZ2	1.84	0.43
1:A:411:GLU:HG3	1:A:412:GLY:N	2.34	0.43
1:A:484:ARG:N	1:A:484:ARG:HD2	2.34	0.43
1:A:125:LEU:N	1:A:126:PRO:CD	2.82	0.43
1:B:293:ASN:H	1:B:293:ASN:ND2	2.04	0.43
1:A:358:LYS:HD3	6:A:923:HOH:O	2.19	0.42
1:B:201:PHE:CZ	1:B:222:GLN:HB2	2.53	0.42
1:B:266:LEU:HG	1:B:267:LYS:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:NE	1:A:108:ARG:HG2	2.35	0.42
1:A:349:ASN:OD1	1:A:359:HIS:CE1	2.72	0.42
1:B:327:ASP:OD1	1:B:329:ALA:HB3	2.20	0.42
1:A:475:ALA:HA	1:A:491:THR:HB	2.02	0.42
1:B:105:TYR:CD2	1:B:228:CYS:SG	3.12	0.42
1:A:378:THR:O	1:A:426:HIS:HB3	2.20	0.41
1:B:119:LEU:O	1:B:122:LEU:HG	2.19	0.41
1:A:140:TYR:CD1	1:A:146:THR:HG22	2.55	0.41
1:A:401:HIS:O	1:A:405:MET:HG2	2.20	0.41
1:B:73:MET:HB3	1:B:78:ARG:HB2	2.01	0.41
1:B:162:ASP:HA	1:B:195:LEU:O	2.21	0.41
1:B:599:GLN:HG2	1:B:601:HIS:O	2.21	0.41
1:B:171:PHE:HD1	1:B:204:GLY:HA3	1.86	0.41
1:B:493:TRP:HH2	1:B:509:VAL:HG13	1.86	0.41
1:A:540:PHE:HA	1:A:543:PHE:HB2	2.02	0.41
1:B:395:GLU:HA	1:B:396:PRO:HD2	1.94	0.41
1:B:180:HIS:CB	1:B:183:ALA:HB2	2.51	0.40
1:A:349:ASN:OD1	1:A:359:HIS:HE1	2.04	0.40
1:A:493:TRP:CH2	1:A:509:VAL:HG13	2.56	0.40
1:B:69:PHE:HD2	1:B:81:ILE:HD13	1.87	0.40
1:A:400:GLU:HG3	1:A:404:LYS:HE3	2.03	0.40
1:B:199:ARG:HH11	1:B:199:ARG:HB3	1.86	0.40
1:B:584:LYS:HD3	1:B:584:LYS:C	2.42	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	603/622 (97%)	586 (97%)	16 (3%)	1 (0%)	47 38
1	B	599/622 (96%)	570 (95%)	28 (5%)	1 (0%)	47 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1202/1244 (97%)	1156 (96%)	44 (4%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	GLY
1	A	141	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	519/531 (98%)	515 (99%)	4 (1%)	81 82
1	B	501/531 (94%)	493 (98%)	8 (2%)	62 60
All	All	1020/1062 (96%)	1008 (99%)	12 (1%)	71 70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	346	MET
1	A	484	ARG
1	A	573	TYR
1	B	212	LEU
1	B	293	ASN
1	B	294	GLN
1	B	346	MET
1	B	358	LYS
1	B	573	TYR
1	B	619	LEU
1	B	646	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	250	HIS
1	A	332	ASN
1	A	359	HIS
1	A	399	GLN
1	A	486	ASN
1	B	96	ASN
1	B	194	GLN
1	B	293	ASN
1	B	294	GLN
1	B	302	HIS
1	B	356	ASN
1	B	467	ASN
1	B	641	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	FMN	B	701	-	33,33,33	2.65	13 (39%)	48,50,50	1.66	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	A	703	-	27,33,52	1.71	5 (18%)	35,52,80	1.63	4 (11%)
4	NAP	B	703	-	30,36,52	1.59	5 (16%)	35,55,80	1.56	3 (8%)
5	PO4	A	704	-	4,4,4	1.67	0	6,6,6	0.44	0
5	PO4	B	704	-	4,4,4	1.61	0	6,6,6	0.43	0
3	FAD	A	702	-	53,58,58	2.13	11 (20%)	68,89,89	1.49	10 (14%)
3	FAD	B	702	-	53,58,58	2.12	11 (20%)	68,89,89	1.50	10 (14%)
2	FMN	A	701	-	33,33,33	2.60	12 (36%)	48,50,50	1.57	12 (25%)

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	FMN	B	701	-	-	0/18/18/18	0/3/3/3
4	NAP	A	703	-	-	1/17/37/67	0/3/3/5
4	NAP	B	703	-	-	5/22/42/67	0/3/3/5
3	FAD	A	702	-	-	2/30/50/50	0/6/6/6
3	FAD	B	702	-	-	1/30/50/50	0/6/6/6
2	FMN	A	701	-	-	0/18/18/18	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C8A-N7A	7.54	1.48	1.34
3	A	702	FAD	C8A-N7A	7.52	1.48	1.34
2	B	701	FMN	C8M-C8	-6.37	1.38	1.51
2	A	701	FMN	C8M-C8	-6.19	1.38	1.51
2	B	701	FMN	C4A-N5	5.87	1.42	1.30
2	A	701	FMN	C4A-N5	5.81	1.42	1.30
3	B	702	FAD	C8M-C8	-5.79	1.39	1.51
3	A	702	FAD	C7M-C7	-5.78	1.39	1.51
3	A	702	FAD	C8M-C8	-5.74	1.39	1.51
3	B	702	FAD	C7M-C7	-5.72	1.39	1.51
2	B	701	FMN	C10-N10	5.26	1.48	1.37
3	A	702	FAD	C2A-N3A	5.15	1.40	1.32
4	A	703	NAP	C2A-N3A	5.13	1.40	1.32
3	B	702	FAD	C2A-N3A	5.11	1.40	1.32
4	B	703	NAP	C2A-N3A	5.10	1.40	1.32
2	B	701	FMN	C9-C9A	4.85	1.47	1.39
2	A	701	FMN	C9-C9A	4.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FMN	C10-N10	4.70	1.47	1.37
2	B	701	FMN	C9A-N10	4.25	1.48	1.41
2	A	701	FMN	C9A-N10	4.25	1.48	1.41
2	A	701	FMN	C9A-C5A	4.11	1.48	1.41
2	B	701	FMN	C9A-C5A	4.04	1.48	1.41
3	A	702	FAD	C9A-N10	-3.86	1.34	1.41
2	B	701	FMN	C8-C7	3.78	1.50	1.40
2	A	701	FMN	C8-C7	3.68	1.50	1.40
3	B	702	FAD	C9A-N10	-3.53	1.34	1.41
3	B	702	FAD	C10-N1	3.51	1.40	1.33
3	A	702	FAD	C10-N1	3.50	1.40	1.33
4	B	703	NAP	C2A-N1A	3.49	1.40	1.33
4	A	703	NAP	C2A-N1A	3.44	1.40	1.33
3	A	702	FAD	C2A-N1A	3.42	1.40	1.33
3	B	702	FAD	C2A-N1A	3.35	1.40	1.33
2	B	701	FMN	C10-N1	3.31	1.40	1.33
2	A	701	FMN	C10-N1	3.08	1.39	1.33
2	A	701	FMN	C6-C5A	2.97	1.44	1.40
2	A	701	FMN	C1'-C2'	2.87	1.56	1.52
4	A	703	NAP	C5A-C4A	-2.75	1.33	1.40
4	B	703	NAP	C5A-C4A	-2.74	1.33	1.40
2	B	701	FMN	C6-C5A	2.73	1.44	1.40
3	A	702	FAD	C5A-C4A	-2.66	1.33	1.40
3	B	702	FAD	C5A-C4A	-2.65	1.33	1.40
2	A	701	FMN	O2'-C2'	2.64	1.48	1.43
3	B	702	FAD	C6A-C5A	-2.64	1.33	1.43
2	B	701	FMN	C4'-C3'	2.63	1.58	1.53
4	A	703	NAP	C6A-C5A	-2.63	1.33	1.43
3	A	702	FAD	C6A-C5A	-2.63	1.33	1.43
4	B	703	NAP	C6A-C5A	-2.60	1.33	1.43
3	A	702	FAD	C5X-N5	-2.56	1.34	1.39
3	B	702	FAD	C5X-N5	-2.52	1.34	1.39
2	B	701	FMN	O2'-C2'	2.47	1.48	1.43
2	A	701	FMN	C4'-C3'	2.38	1.58	1.53
2	B	701	FMN	C1'-C2'	2.29	1.55	1.52
3	B	702	FAD	O4B-C1B	2.23	1.44	1.41
4	B	703	NAP	O4B-C1B	2.18	1.44	1.41
3	A	702	FAD	O4B-C1B	2.15	1.44	1.41
4	A	703	NAP	O4B-C1B	2.12	1.44	1.41
2	B	701	FMN	C7M-C7	2.03	1.55	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N3A-C2A-N1A	-7.19	117.45	128.68
3	B	702	FAD	N3A-C2A-N1A	-7.17	117.47	128.68
4	A	703	NAP	N3A-C2A-N1A	-7.03	117.70	128.68
4	B	703	NAP	N3A-C2A-N1A	-6.89	117.90	128.68
2	B	701	FMN	C9A-C5A-N5	4.05	126.84	122.43
2	A	701	FMN	C9A-C5A-N5	3.84	126.61	122.43
2	B	701	FMN	P-O5'-C5'	3.62	128.26	118.30
2	A	701	FMN	O4'-C4'-C3'	-3.49	100.61	109.10
2	B	701	FMN	O4'-C4'-C3'	-3.40	100.84	109.10
3	B	702	FAD	C4-N3-C2	-3.02	120.06	125.64
2	A	701	FMN	P-O5'-C5'	2.91	126.31	118.30
3	A	702	FAD	C4-N3-C2	-2.83	120.41	125.64
2	B	701	FMN	O4-C4-N3	-2.82	114.71	120.12
3	B	702	FAD	C5A-C6A-N6A	-2.81	116.08	120.35
3	A	702	FAD	C5A-C6A-N6A	-2.79	116.11	120.35
3	B	702	FAD	P-O3P-PA	-2.79	123.26	132.83
3	B	702	FAD	C4X-C4-N3	2.79	120.27	113.19
3	A	702	FAD	P-O3P-PA	-2.77	123.34	132.83
3	A	702	FAD	C4X-C4-N3	2.67	119.97	113.19
3	B	702	FAD	C10-C4X-N5	-2.67	119.20	124.86
3	A	702	FAD	C10-C4X-N5	-2.61	119.31	124.86
2	B	701	FMN	O3P-P-O5'	-2.60	99.81	106.73
2	A	701	FMN	C8M-C8-C7	2.57	126.00	120.74
2	A	701	FMN	O4-C4-N3	-2.55	115.23	120.12
2	A	701	FMN	C5A-N5-C4A	-2.53	113.87	118.07
4	A	703	NAP	C3B-C2B-C1B	-2.52	98.14	102.89
2	B	701	FMN	C8M-C8-C7	2.50	125.86	120.74
2	B	701	FMN	C5A-C9A-N10	-2.40	115.48	117.95
2	B	701	FMN	C5A-N5-C4A	-2.38	114.11	118.07
4	B	703	NAP	C3B-C2B-C1B	-2.37	98.43	102.89
3	B	702	FAD	O4-C4-C4X	-2.32	120.44	126.60
2	B	701	FMN	O2P-P-O1P	2.30	119.67	110.68
3	A	702	FAD	C9A-C5X-N5	-2.26	119.97	122.43
3	B	702	FAD	C2B-C3B-C4B	-2.26	98.25	102.64
2	A	701	FMN	O2P-P-O1P	2.25	119.48	110.68
3	A	702	FAD	O4-C4-C4X	-2.24	120.65	126.60
2	B	701	FMN	C9-C9A-N10	2.23	124.85	121.84
3	A	702	FAD	C2B-C3B-C4B	-2.22	98.32	102.64
2	A	701	FMN	C8M-C8-C9	-2.17	115.47	119.49
3	B	702	FAD	C4X-C10-N10	2.13	119.60	116.48
2	B	701	FMN	C4'-C3'-C2'	-2.10	109.00	113.36
2	A	701	FMN	C4'-C3'-C2'	-2.09	109.01	113.36
2	B	701	FMN	C7M-C7-C6	-2.08	115.64	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FMN	C5A-C9A-N10	-2.08	115.81	117.95
4	A	703	NAP	C5A-C6A-N6A	-2.08	117.19	120.35
3	B	702	FAD	C9A-C5X-N5	-2.07	120.18	122.43
4	B	703	NAP	C5A-C6A-N6A	-2.06	117.22	120.35
4	A	703	NAP	O2N-PN-O1N	2.06	118.73	110.68
3	A	702	FAD	C4X-C10-N10	2.05	119.47	116.48
2	B	701	FMN	C8M-C8-C9	-2.03	115.73	119.49
2	A	701	FMN	O3P-P-O5'	-2.01	101.39	106.73
2	A	701	FMN	C7M-C7-C6	-2.01	115.78	119.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

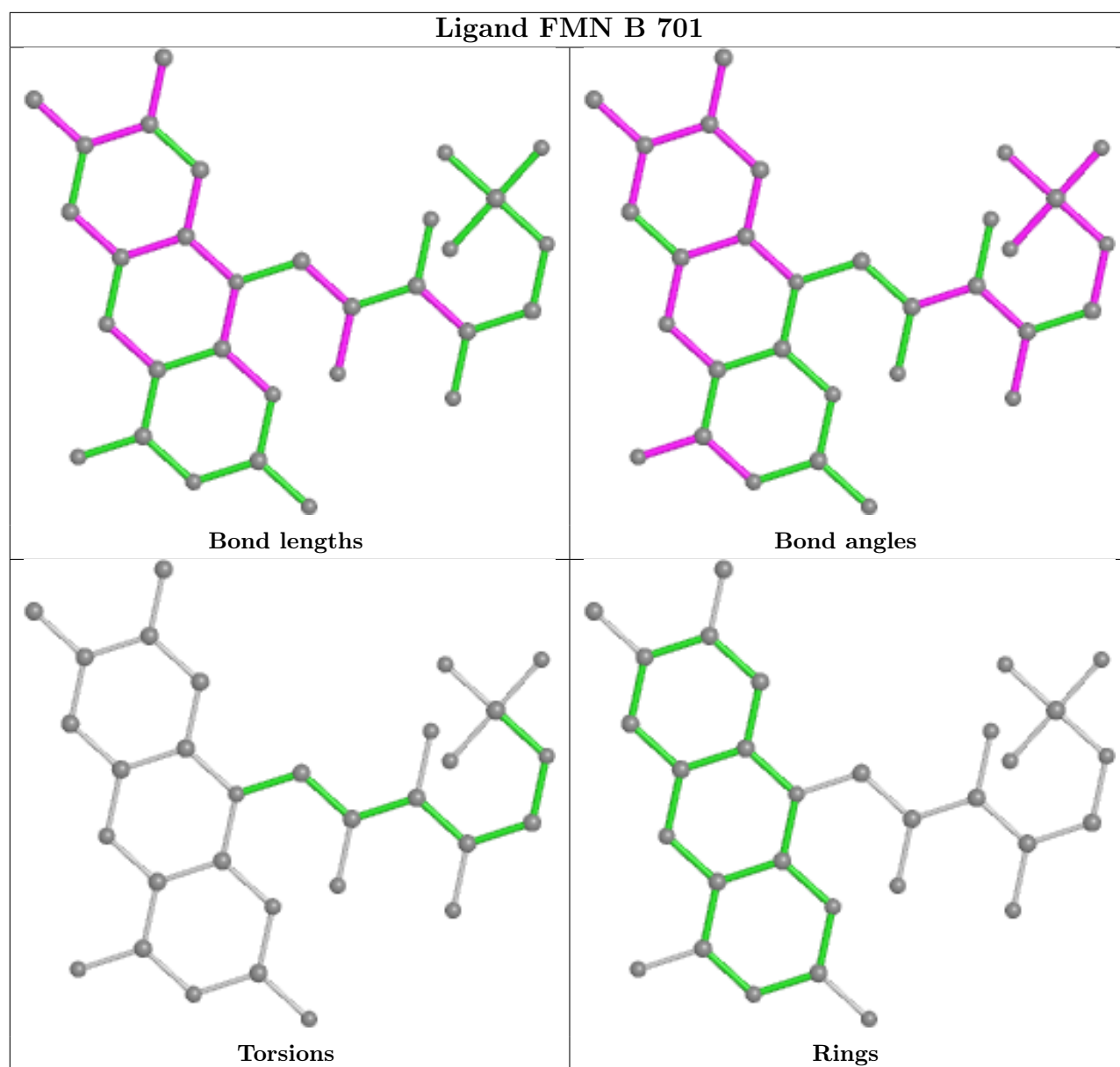
Mol	Chain	Res	Type	Atoms
4	B	703	NAP	C5D-O5D-PN-O1N
4	B	703	NAP	C5D-O5D-PN-O2N
4	B	703	NAP	C3D-C4D-C5D-O5D
3	A	702	FAD	PA-O3P-P-O1P
4	A	703	NAP	C2B-O2B-P2B-O3X
4	B	703	NAP	C2B-O2B-P2B-O3X
4	B	703	NAP	C5D-O5D-PN-O3
3	A	702	FAD	PA-O3P-P-O2P
3	B	702	FAD	PA-O3P-P-O2P

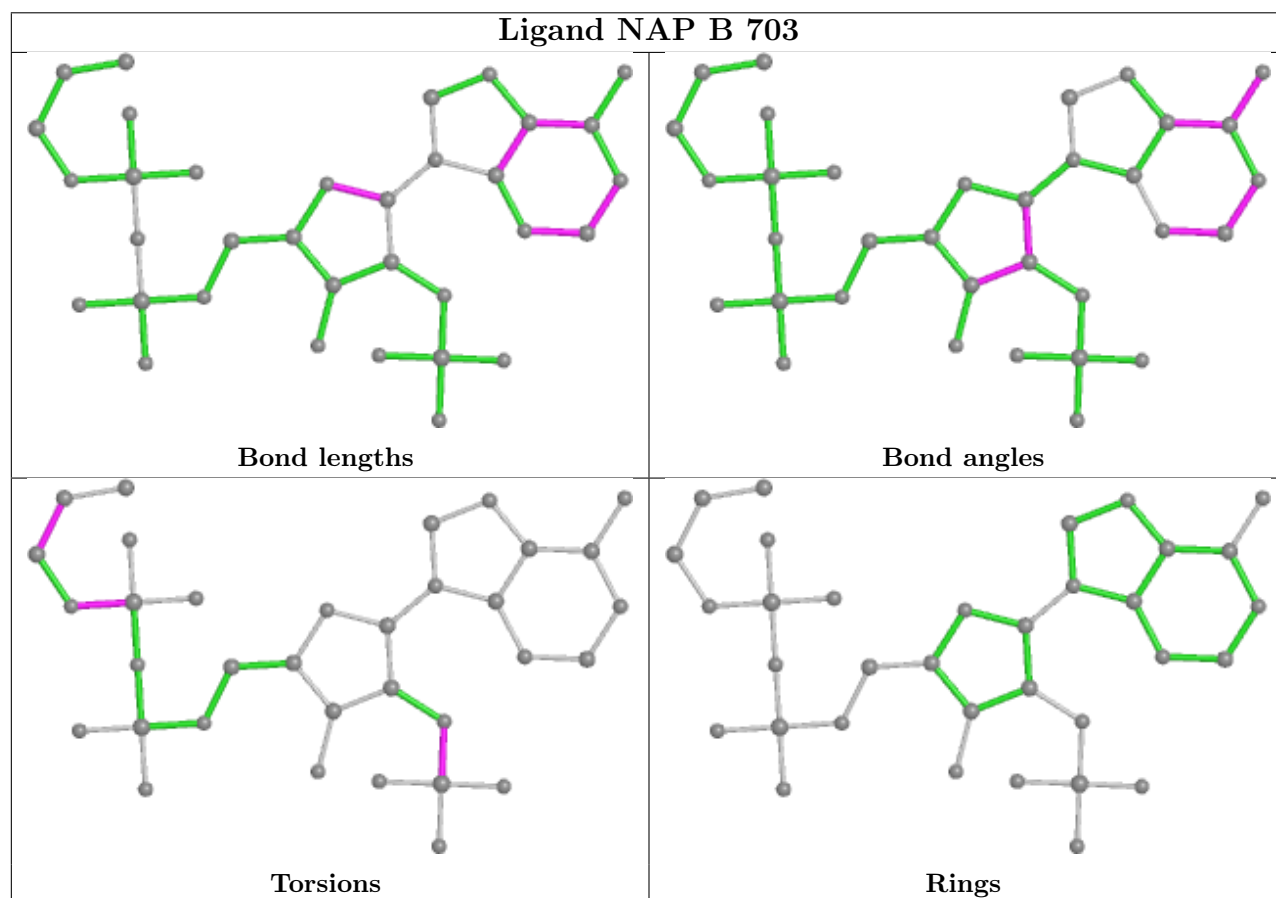
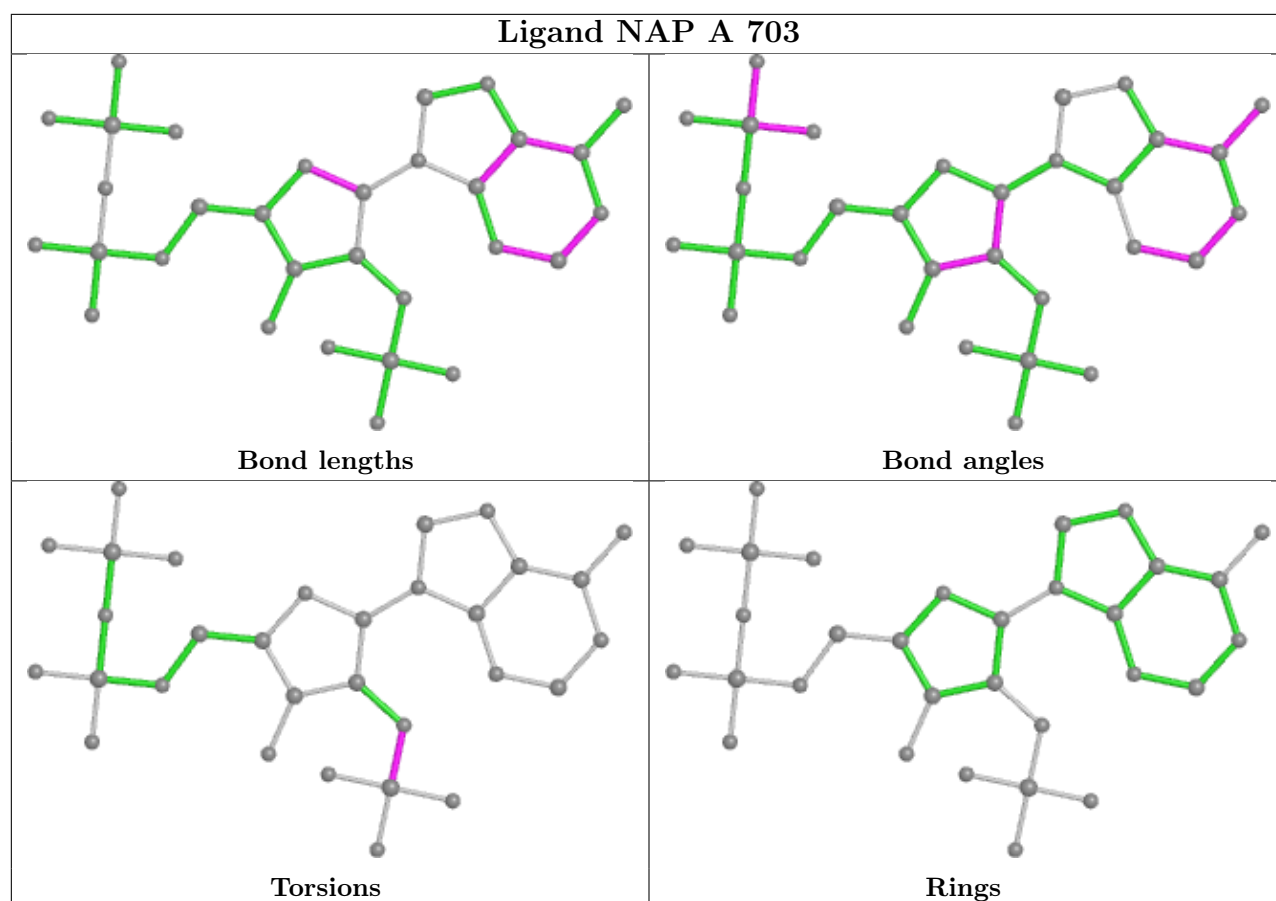
There are no ring outliers.

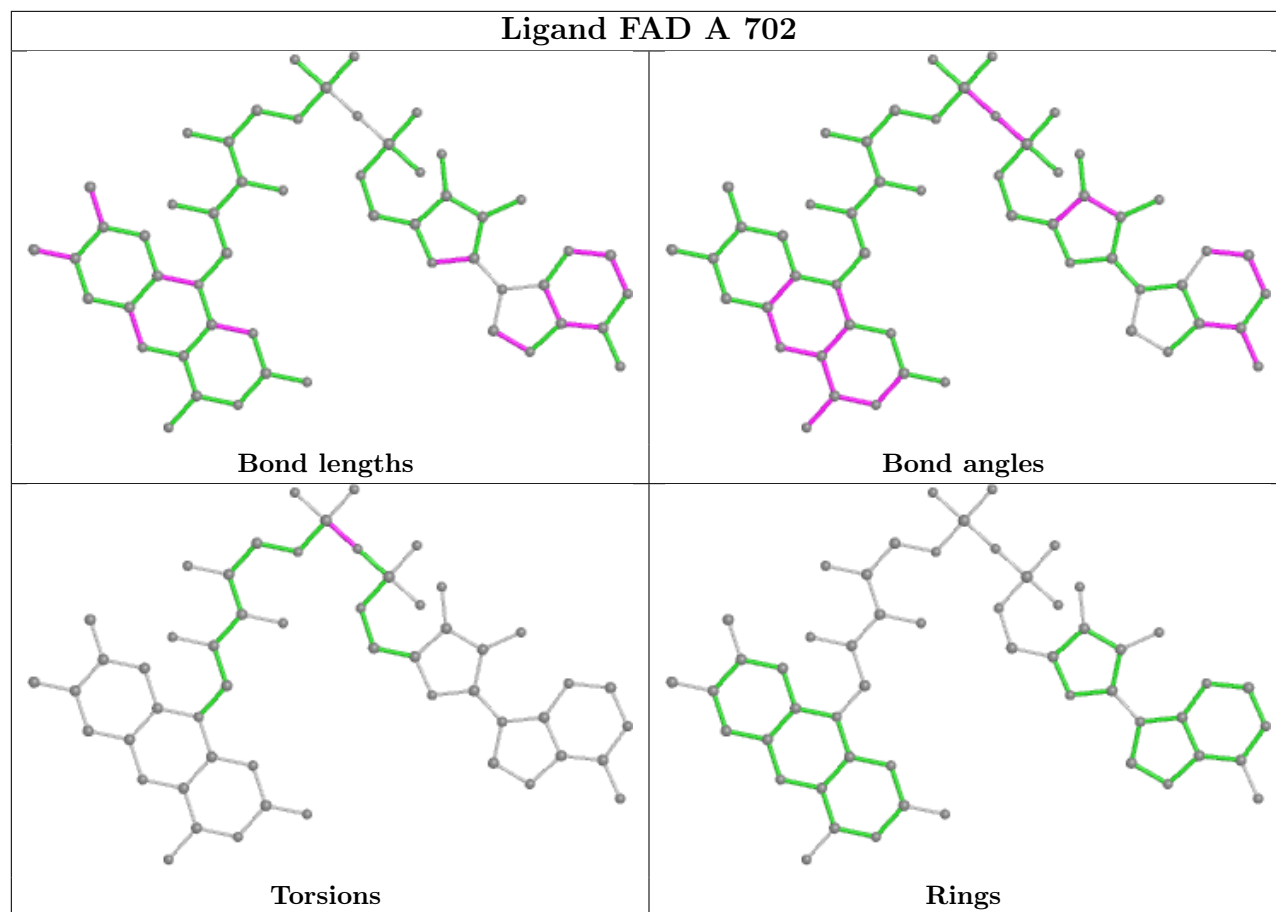
1 monomer is involved in 2 short contacts:

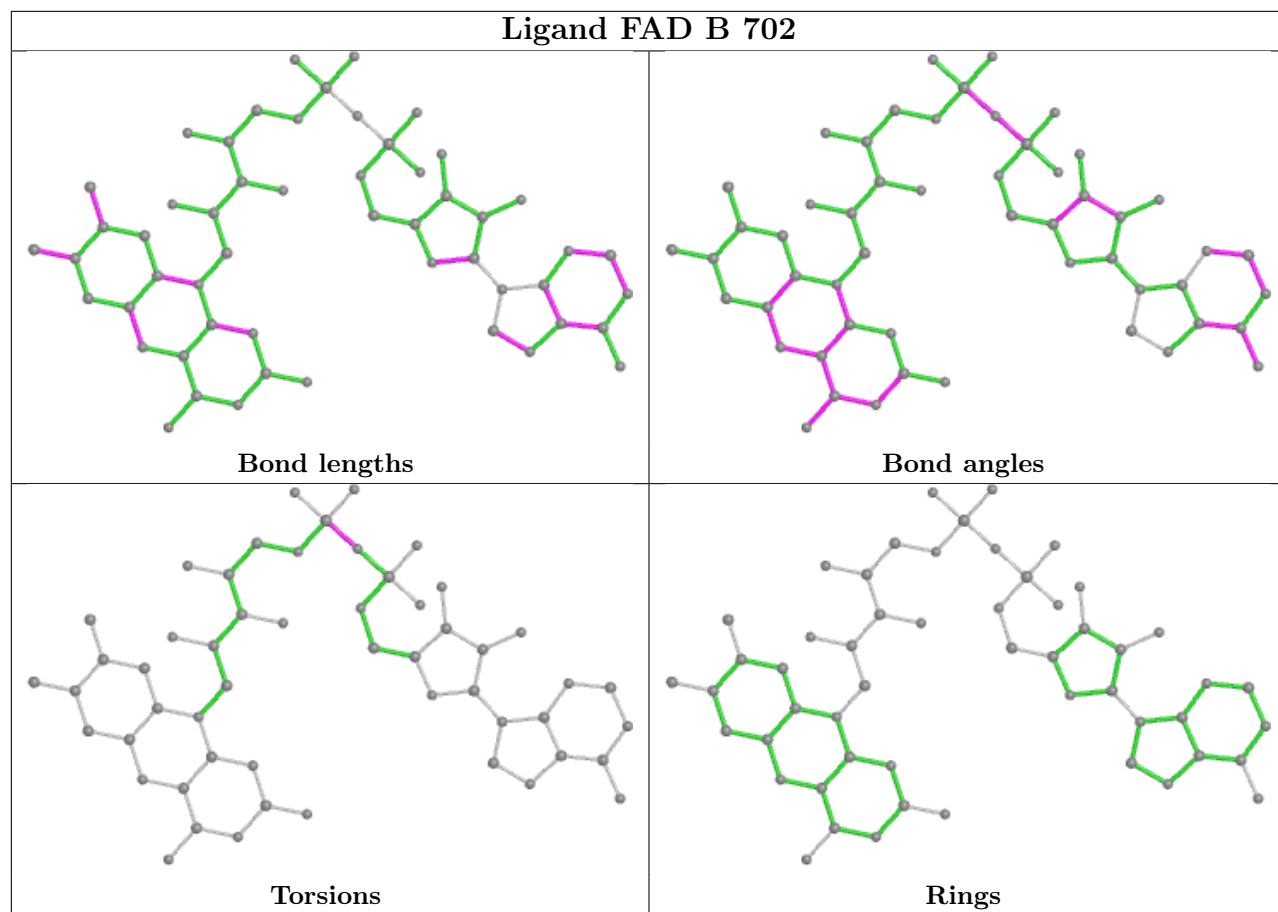
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FMN	2	0

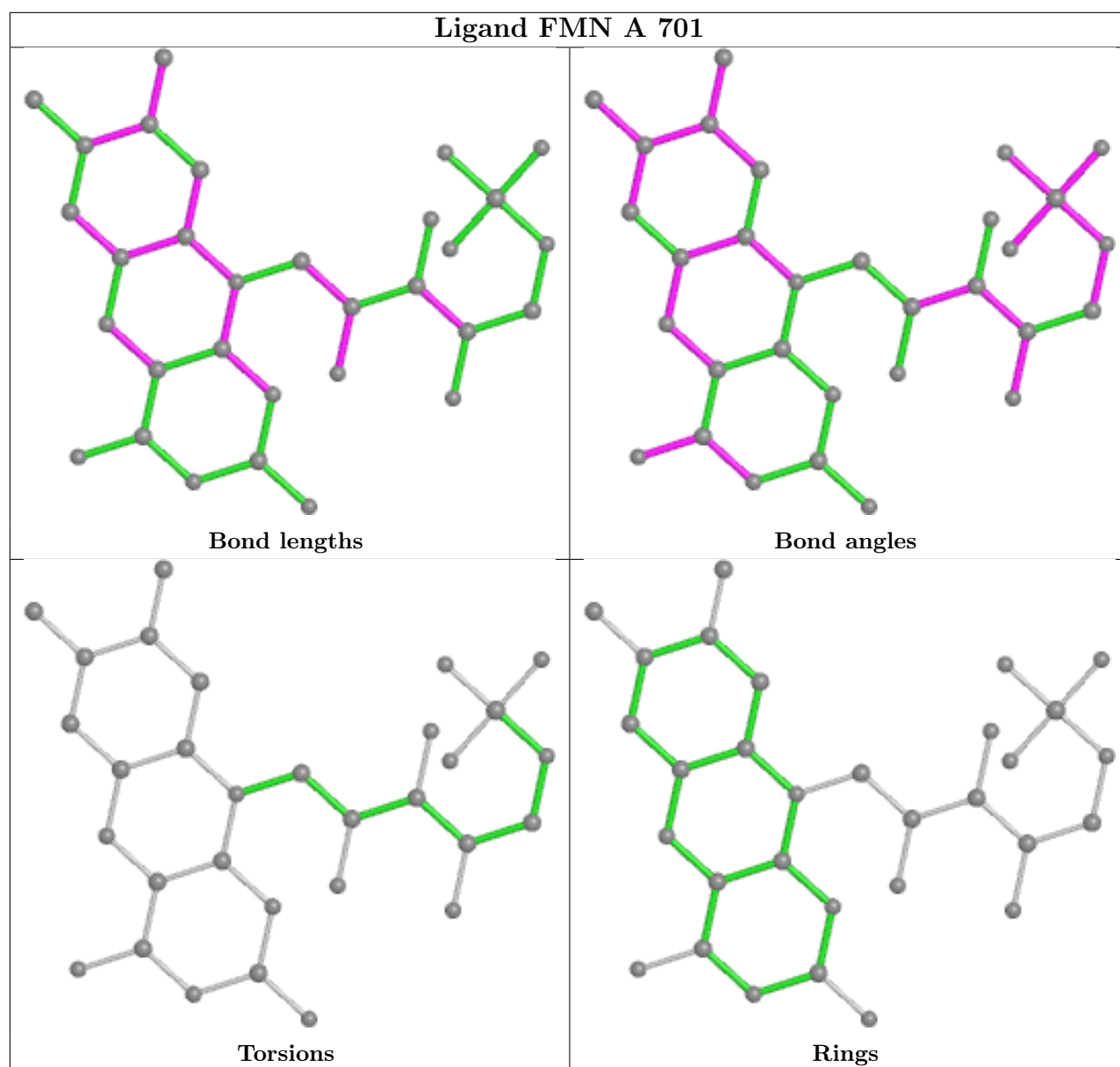
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	609/622 (97%)	0.07	11 (1%) 68 71	23, 34, 52, 72	0
1	B	605/622 (97%)	0.82	93 (15%) 2 2	22, 40, 91, 97	0
All	All	1214/1244 (97%)	0.44	104 (8%) 10 12	22, 36, 84, 97	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	PHE	8.8
1	B	156	LEU	8.4
1	B	161	VAL	7.4
1	B	233	VAL	7.3
1	B	200	ILE	7.2
1	B	125	LEU	6.9
1	B	235	ALA	6.6
1	B	163	LEU	6.3
1	B	106	GLY	6.3
1	B	228	CYS	6.2
1	B	119	LEU	6.2
1	B	166	VAL	6.2
1	B	192	LEU	6.1
1	B	64	VAL	6.1
1	B	105	TYR	5.6
1	B	169	ALA	5.5
1	B	224	TRP	5.5
1	B	164	THR	5.4
1	B	227	VAL	5.4
1	B	69	PHE	5.3
1	A	500	ALA	5.2
1	B	162	ASP	5.1
1	B	232	GLY	5.0
1	B	71	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	124	SER	4.9
1	B	155	TRP	4.7
1	B	187	TYR	4.7
1	B	135	PHE	4.5
1	B	83	PHE	4.3
1	B	168	PHE	4.3
1	B	195	LEU	4.2
1	A	252	ASP	4.1
1	B	103	HIS	4.1
1	B	77	GLY	4.0
1	B	236	THR	4.0
1	B	120	ALA	4.0
1	B	198	GLN	3.8
1	B	201	PHE	3.8
1	B	141	GLY	3.7
1	B	104	ARG	3.6
1	B	122	LEU	3.5
1	B	165	GLY	3.5
1	B	81	ILE	3.4
1	B	108	ARG	3.4
1	B	134	VAL	3.4
1	B	205	LEU	3.4
1	B	229	GLU	3.3
1	B	191	ARG	3.3
1	B	181	PHE	3.3
1	B	76	THR	3.3
1	B	225	PRO	3.3
1	B	189	ASP	3.2
1	B	129	ASP	3.2
1	B	131	SER	3.2
1	B	128	ILE	3.2
1	A	240	SER	3.1
1	A	141	GLY	3.1
1	B	180	HIS	3.0
1	B	234	GLU	3.0
1	A	506	ARG	3.0
1	B	242	ILE	3.0
1	B	80	ILE	2.9
1	B	102	ALA	2.9
1	B	78	ARG	2.9
1	B	254	ASP	2.9
1	A	254	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	351	LEU	2.8
1	A	251	GLU	2.8
1	B	179	GLU	2.7
1	B	414	GLU	2.7
1	B	223	PHE	2.6
1	B	167	LYS	2.6
1	B	107	MET	2.6
1	B	184	MET	2.6
1	B	202	GLU	2.6
1	B	75	LYS	2.5
1	B	117	TYR	2.5
1	B	160	ASP	2.4
1	B	217	ILE	2.4
1	B	176	LYS	2.4
1	A	253	MET	2.4
1	B	313	ARG	2.4
1	A	140	TYR	2.4
1	B	140	TYR	2.4
1	B	100	LYS	2.4
1	B	178	TYR	2.3
1	B	209	ASP	2.3
1	B	143	GLY	2.3
1	B	127	GLU	2.3
1	B	136	CYS	2.2
1	A	255	VAL	2.2
1	B	153	TYR	2.2
1	B	157	GLN	2.2
1	B	190	GLN	2.2
1	B	170	VAL	2.2
1	B	222	GLN	2.1
1	B	72	LYS	2.1
1	B	110	MET	2.1
1	A	297	GLU	2.1
1	B	73	MET	2.1
1	B	121	ASP	2.0
1	B	68	SER	2.0
1	B	207	ASP	2.0
1	B	203	LEU	2.0

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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

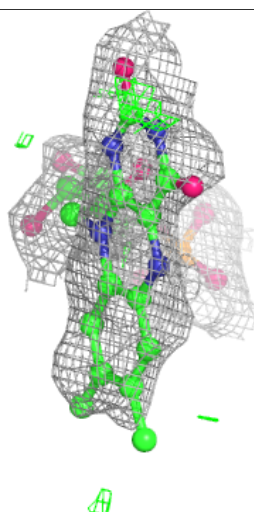
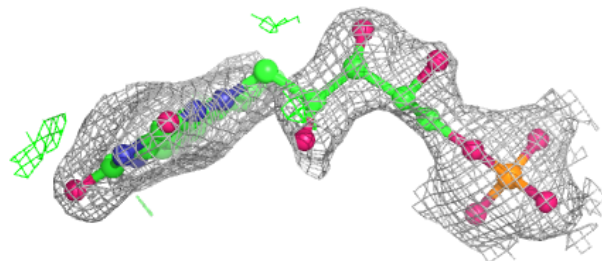
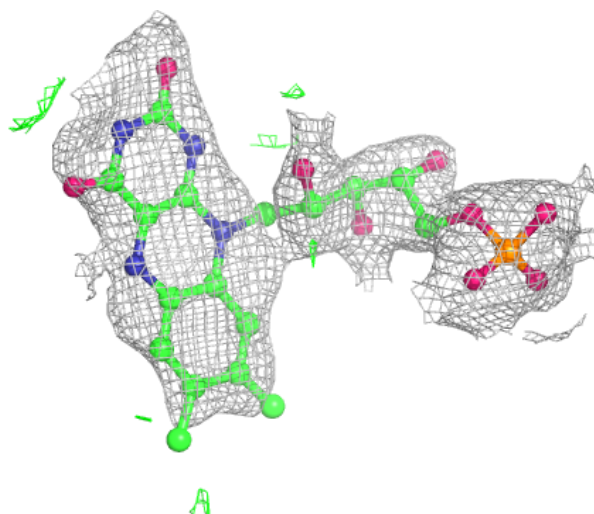
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	A	704	5/5	0.81	0.27	108,109,109,109	0
2	FMN	B	701	31/31	0.90	0.17	52,67,69,70	0
4	NAP	B	703	34/48	0.94	0.15	23,27,68,77	0
5	PO4	B	704	5/5	0.94	0.14	58,61,62,63	0
2	FMN	A	701	31/31	0.95	0.13	31,37,43,43	0
4	NAP	A	703	31/48	0.97	0.12	25,27,52,55	0
3	FAD	A	702	53/53	0.97	0.12	22,26,36,37	0
3	FAD	B	702	53/53	0.98	0.12	18,23,34,37	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.

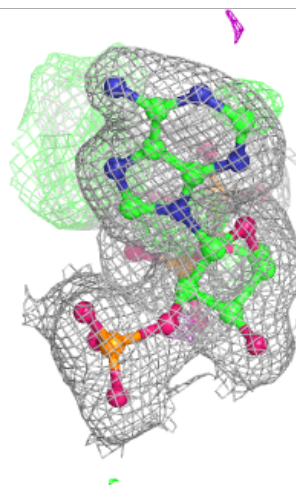
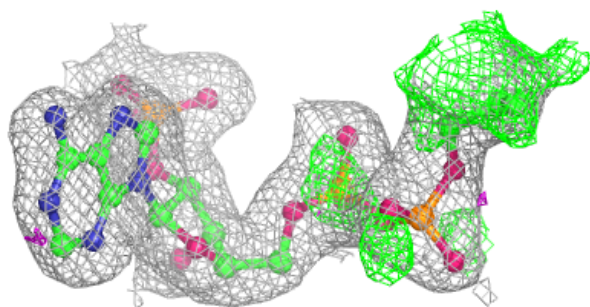
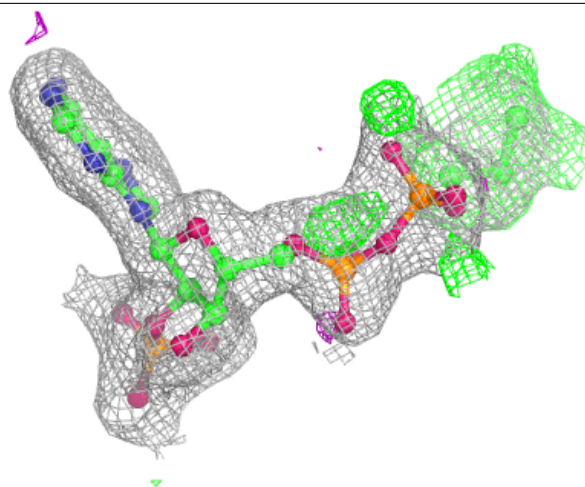
Electron density around FMN B 701:

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



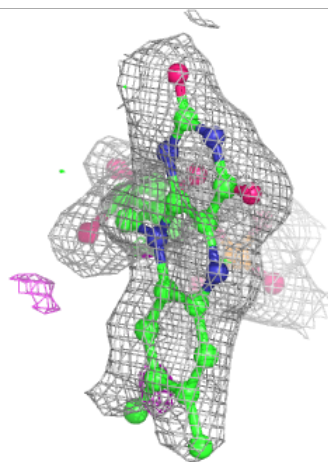
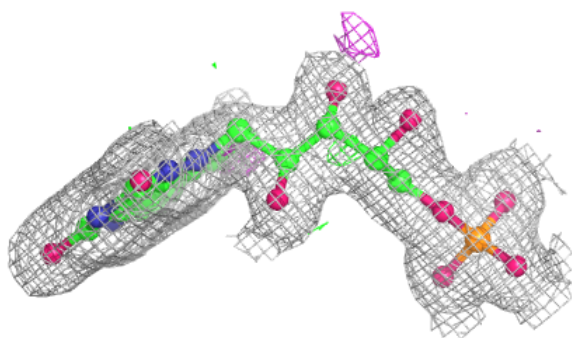
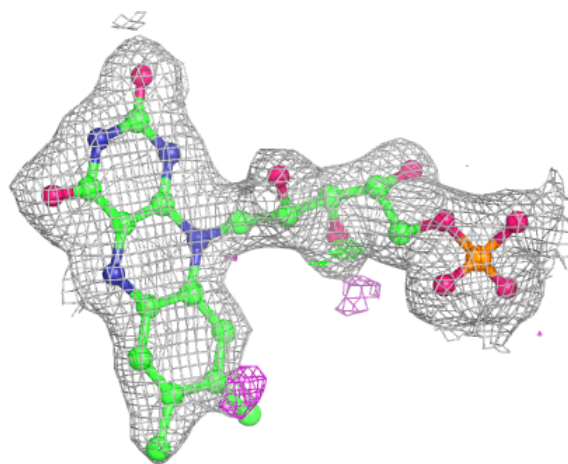
Electron density around NAP B 703:

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



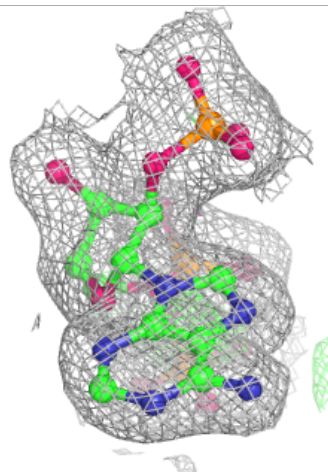
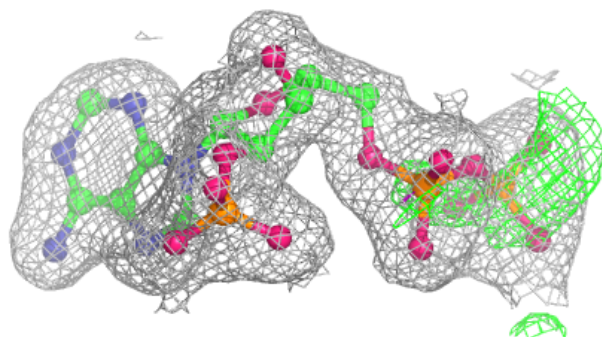
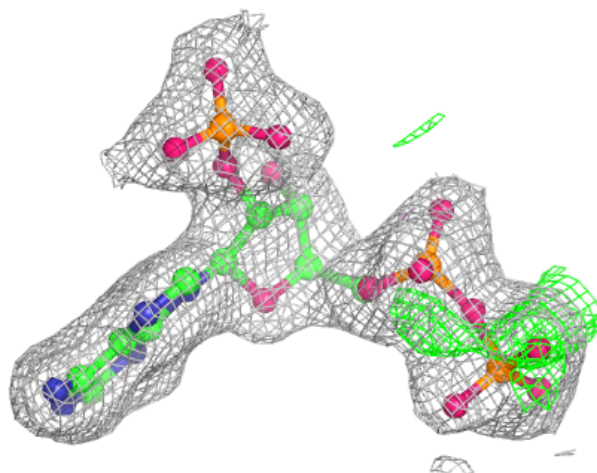
Electron density around FMN A 701:

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



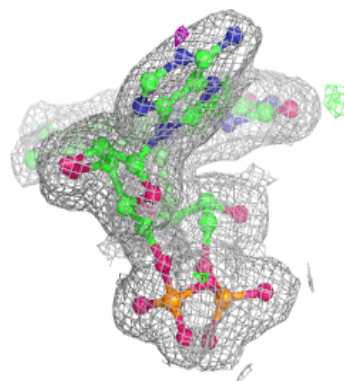
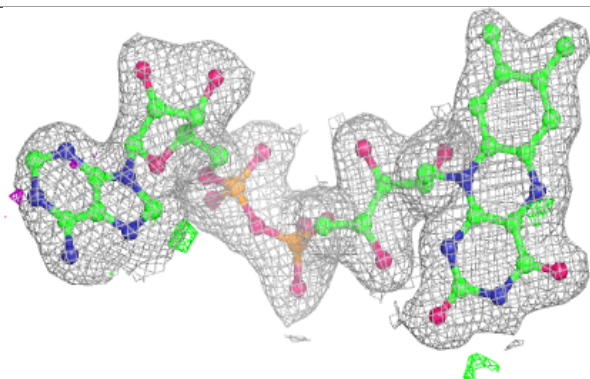
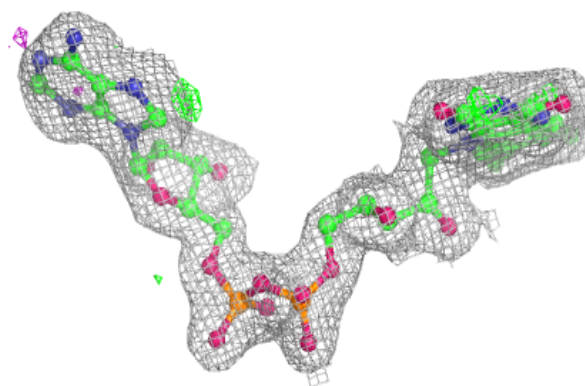
Electron density around NAP A 703:

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

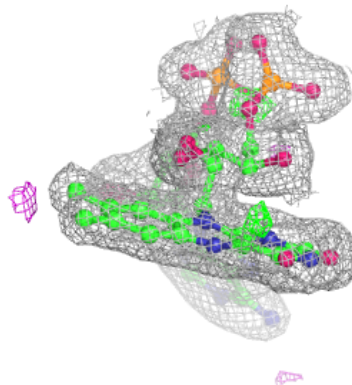
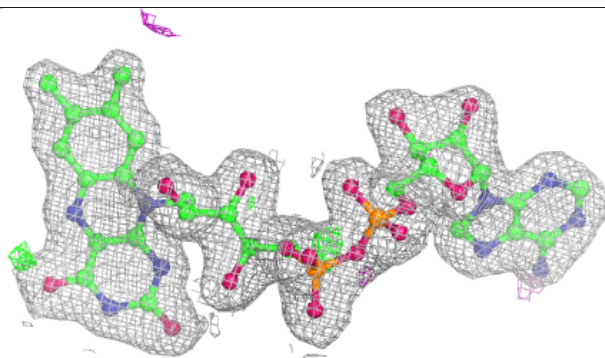
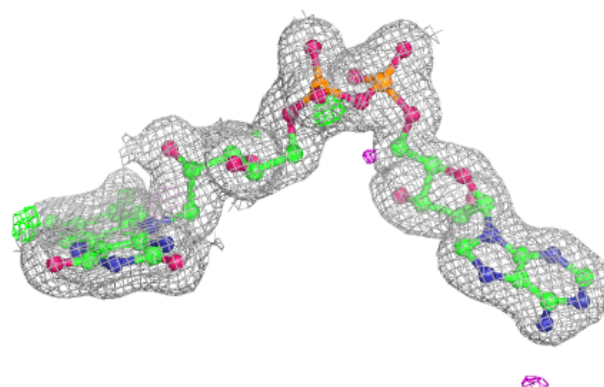


Electron density around FAD A 702:

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

**Electron density around FAD B 702:**

$2mF_o-DF_c$ (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.