



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:00 AM UTC

PDB ID : 5URH / pdb_00005urh
Title : CYPOR/D632A with NADP+
Authors : Xia, C.; Kim, J.J.
Deposited on : 2017-02-10
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

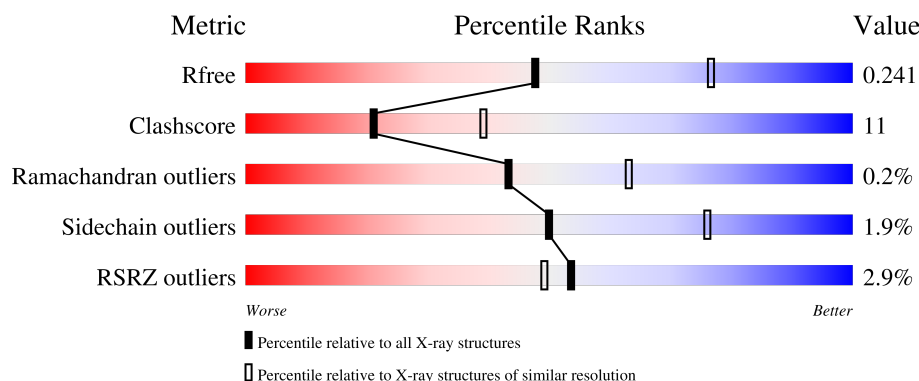
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10276 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.

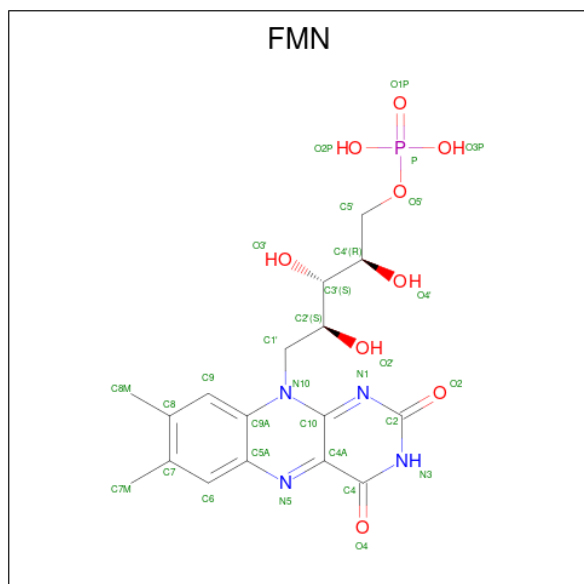
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4860	3084	833	920	23			
1	B	606	Total	C	N	O	S	0	0	1
			4822	3060	830	909	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	632	ALA	ASP	engineered mutation	UNP P00388
B	632	ALA	ASP	engineered mutation	UNP P00388

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



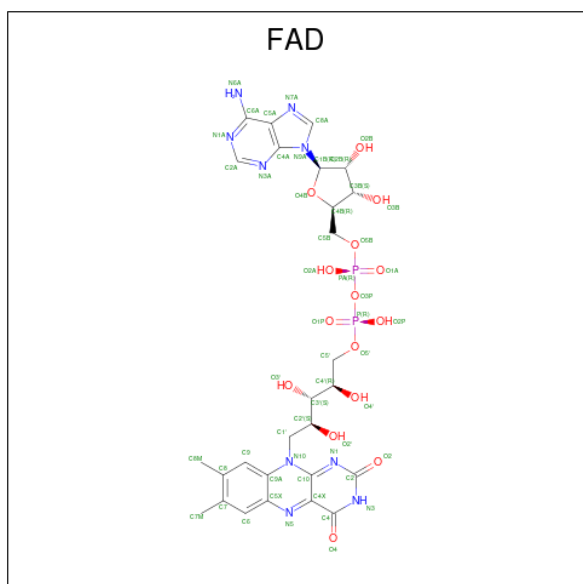
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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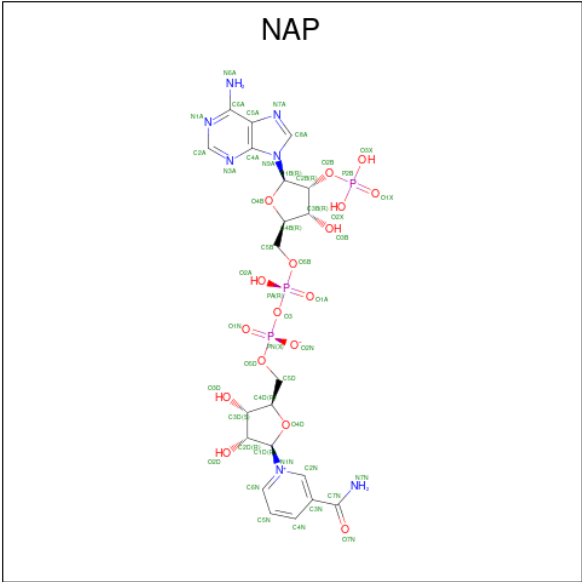
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



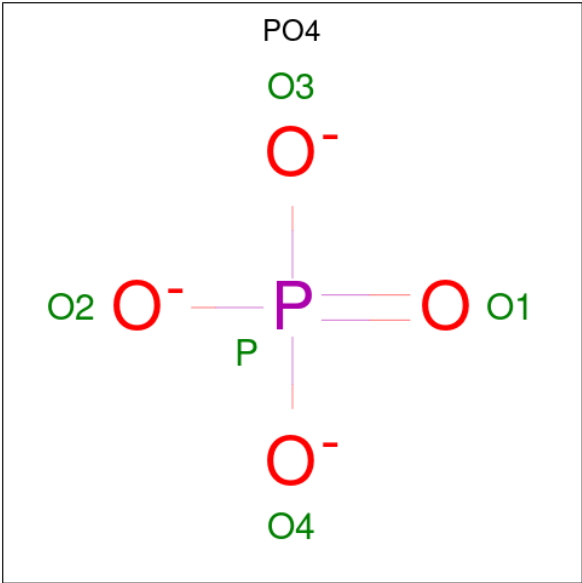
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 40	C 15	N 6	O 16	P 3	0	0
4	B	1	Total 40	C 15	N 6	O 16	P 3	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: 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		

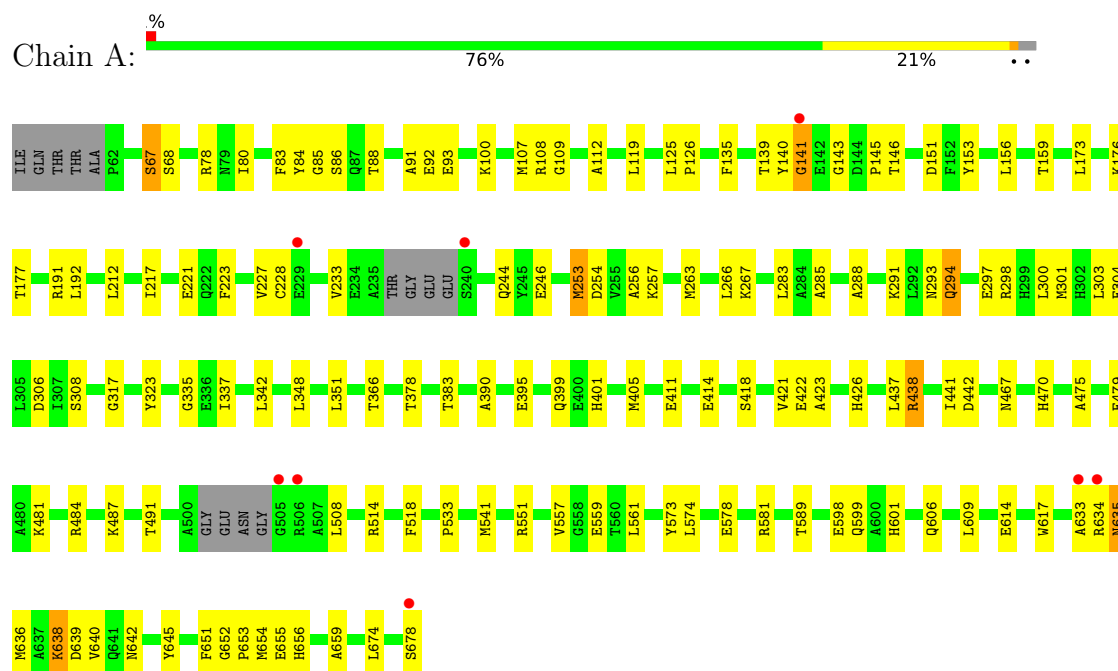
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	180	Total 180	O 180	0	0
6	B	156	Total 156	O 156	0	0

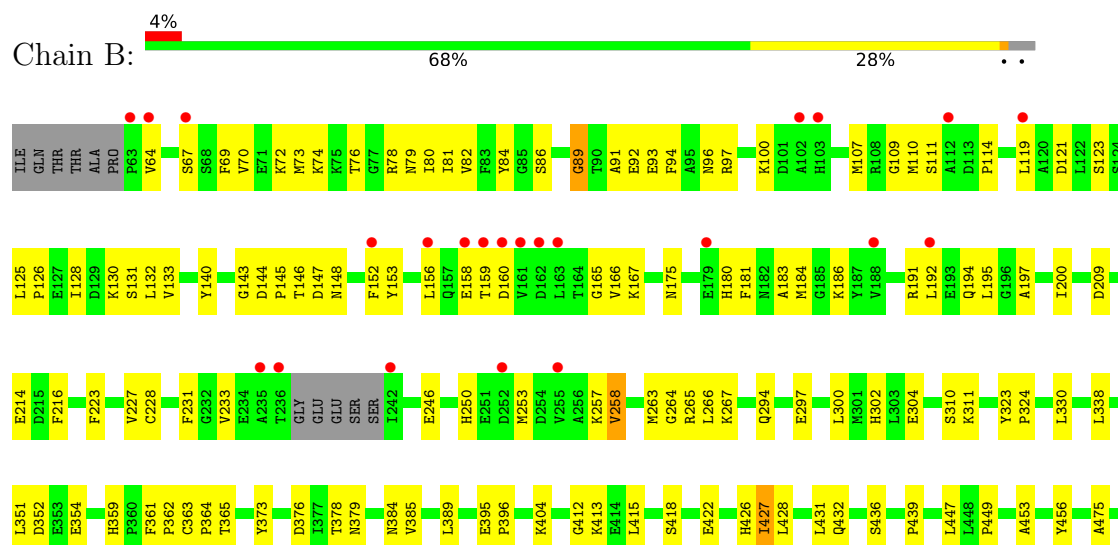
3 Residue-property plots

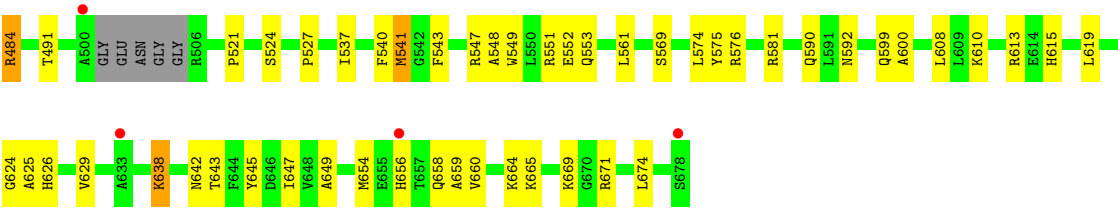
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	101.68Å 116.21Å 118.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.95 – 2.50 46.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.95-2.50) 99.9 (46.95-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.48Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.204 , 0.251 0.198 , 0.241	Depositor DCC
R_{free} test set	2465 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10276	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.33% 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: PO4, NAP, FMN, 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	0.44	0/4975	0.90	13/6729 (0.2%)
1	B	0.41	0/4937	0.94	15/6681 (0.2%)
All	All	0.43	0/9912	0.92	28/13410 (0.2%)

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	B	0	1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	GLU	N-CA-C	13.65	130.63	113.43
1	B	158	GLU	CB-CA-C	-9.52	93.65	109.65
1	B	159	THR	CB-CA-C	-7.18	96.45	109.38
1	B	160	ASP	N-CA-CB	-6.75	100.85	111.39
1	A	395	GLU	CA-C-N	6.11	125.59	119.24
1	A	395	GLU	C-N-CA	6.11	125.59	119.24
1	B	89	GLY	N-CA-C	6.07	123.41	115.40
1	A	438	ARG	CA-C-N	5.89	123.90	119.66
1	A	438	ARG	C-N-CA	5.89	123.90	119.66
1	B	415	LEU	N-CA-C	-5.86	104.81	111.14
1	A	655	GLU	N-CA-C	-5.79	101.44	110.42
1	B	67	SER	N-CA-CB	-5.74	102.46	110.38
1	A	159	THR	N-CA-C	5.73	117.93	110.43
1	B	524	SER	N-CA-C	5.61	119.61	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	MET	N-CA-C	-5.51	105.42	111.82
1	A	541	MET	N-CA-C	-5.51	105.42	111.82
1	B	427	ILE	N-CA-C	5.44	116.17	110.62
1	B	258	VAL	N-CA-C	5.37	116.05	108.36
1	B	67	SER	N-CA-C	5.37	117.76	110.35
1	A	146	THR	N-CA-C	-5.35	103.47	110.53
1	A	85	GLY	N-CA-C	-5.33	100.56	113.18
1	A	253	MET	N-CA-C	5.30	116.67	107.93
1	A	176	LYS	N-CA-C	5.24	117.74	111.71
1	A	301	MET	N-CA-C	5.22	117.75	109.50
1	B	297	GLU	N-CA-C	-5.14	105.68	111.28
1	A	421	VAL	N-CA-C	5.12	115.24	110.42
1	B	72	LYS	N-CA-C	-5.07	105.94	111.82
1	B	373	TYR	N-CA-C	5.04	120.43	113.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	456	TYR	Sidechain

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	4860	0	4703	83	0
1	B	4822	0	4652	130	0
2	A	31	0	19	1	0
2	B	31	0	19	0	0
3	A	53	0	31	1	0
3	B	53	0	31	0	0
4	A	40	0	19	3	0
4	B	40	0	19	0	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
6	A	180	0	0	4	0
6	B	156	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10276	0	9493	213	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 11.

All (213) 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:86:SER:HB2	1:B:91:ALA:HB3	1.46	0.93
1:A:639:ASP:C	1:A:640:VAL:CA	2.42	0.93
1:B:70:VAL:HG23	1:B:121:ASP:HB3	1.57	0.86
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.60	0.84
1:A:633:ALA:HB3	1:A:678:SER:HA	1.60	0.83
1:A:294:GLN:H	1:A:294:GLN:NE2	1.81	0.79
1:B:107:MET:HE2	1:B:233:VAL:HG21	1.65	0.77
1:A:254:ASP:HB2	1:A:257:LYS:HE2	1.67	0.77
1:B:181:PHE:O	1:B:186:LYS:HE2	1.87	0.74
1:B:191:ARG:O	1:B:195:LEU:HD13	1.89	0.71
1:B:119:LEU:HG	1:B:152:PHE:CD1	2.28	0.69
1:A:411:GLU:HA	1:A:414:GLU:OE1	1.93	0.68
1:B:385:VAL:HG13	1:B:447:LEU:HB3	1.74	0.68
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.74	0.67
1:A:559:GLU:HG2	1:A:589:THR:HG21	1.77	0.65
1:A:300:LEU:HD22	1:A:574:LEU:HD21	1.78	0.65
1:B:152:PHE:O	1:B:156:LEU:HG	1.96	0.64
1:B:97:ARG:HH21	1:B:384:ASN:HB3	1.63	0.64
1:B:145:PRO:HG2	1:B:153:TYR:CG	2.33	0.63
1:B:192:LEU:O	1:B:197:ALA:HB3	1.98	0.63
1:A:93:GLU:OE1	1:A:93:GLU:HA	1.97	0.63
1:B:228:CYS:HA	1:B:233:VAL:HG22	1.81	0.63
1:B:615:HIS:O	1:B:619:LEU:HD13	1.99	0.63
1:B:80:ILE:O	1:B:109:GLY:HA2	1.98	0.62
1:B:97:ARG:NH2	1:B:384:ASN:HB3	2.14	0.62
1:B:93:GLU:O	1:B:97:ARG:HG3	1.99	0.62
1:B:418:SER:O	1:B:422:GLU:HB3	1.99	0.61
1:B:250:HIS:HB3	1:B:253:MET:HB2	1.83	0.61
1:B:629:VAL:HB	1:B:674:LEU:HD23	1.81	0.60
1:B:302:HIS:HD2	1:B:575:TYR:OH	1.85	0.60
1:A:253:MET:HG3	1:A:257:LYS:HE3	1.83	0.60
1:B:107:MET:HE1	1:B:227:VAL:HG12	1.83	0.59
1:A:285:ALA:HA	1:A:508:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.86	0.57
1:B:246:GLU:HB3	1:B:351:LEU:HD21	1.86	0.57
1:B:638:LYS:HA	1:B:638:LYS:HE3	1.85	0.57
1:A:390:ALA:O	1:A:399:GLN:HG3	2.05	0.57
1:B:300:LEU:HD22	1:B:574:LEU:HD21	1.87	0.56
1:B:656:HIS:O	1:B:660:VAL:HG23	2.05	0.56
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.88	0.56
1:B:223:PHE:O	1:B:227:VAL:HG23	2.05	0.56
1:B:214:GLU:OE1	1:B:413:LYS:HE3	2.04	0.56
1:B:624:GLY:HA2	1:B:671:ARG:NH2	2.20	0.56
1:B:175:ASN:OD1	1:B:209:ASP:HB2	2.06	0.55
1:B:549:TRP:O	1:B:553:GLN:HG2	2.06	0.55
1:B:266:LEU:O	1:B:267:LYS:HB2	2.05	0.55
1:B:228:CYS:HA	1:B:233:VAL:CG2	2.37	0.55
1:B:642:ASN:HA	1:B:645:TYR:CD2	2.42	0.55
1:A:139:THR:CG2	1:A:143:GLY:HA2	2.37	0.54
1:A:139:THR:HG21	1:A:143:GLY:HA2	1.89	0.54
1:B:359:HIS:ND1	1:B:363:CYS:HB2	2.22	0.54
1:B:81:ILE:HG13	1:B:110:MET:O	2.07	0.54
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.38	0.54
1:A:606:GLN:OE1	4:A:703:NAP:H2A	2.08	0.54
1:B:561:LEU:CD2	1:B:590:GLN:HB2	2.36	0.53
1:B:167:LYS:HB3	1:B:200:ILE:HD13	1.89	0.53
1:B:228:CYS:HB3	1:B:233:VAL:O	2.09	0.53
1:B:548:ALA:O	1:B:552:GLU:HG3	2.07	0.53
1:A:475:ALA:HA	1:A:491:THR:HB	1.91	0.53
1:A:634:ARG:O	1:A:638:LYS:HG2	2.09	0.53
1:B:133:VAL:O	1:B:133:VAL:HG13	2.09	0.53
1:A:135:PHE:CE2	1:A:192:LEU:HD11	2.44	0.52
1:A:437:LEU:O	1:A:438:ARG:HD3	2.10	0.52
1:B:119:LEU:HG	1:B:152:PHE:HD1	1.72	0.52
1:B:228:CYS:SG	1:B:233:VAL:HG23	2.50	0.52
1:B:654:MET:HB2	1:B:658:GLN:HB2	1.92	0.52
1:B:404:LYS:HD2	1:B:412:GLY:HA3	1.92	0.51
1:B:428:LEU:O	1:B:432:GLN:HG3	2.10	0.51
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.91	0.51
1:B:82:VAL:O	1:B:111:SER:HA	2.10	0.51
1:B:257:LYS:O	1:B:257:LYS:HG2	2.10	0.51
1:A:223:PHE:O	1:A:227:VAL:HG23	2.11	0.51
1:B:123:SER:O	1:B:126:PRO:HD2	2.10	0.51
1:B:128:ILE:O	1:B:131:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:LEU:HD12	1:B:619:LEU:N	2.26	0.50
1:B:145:PRO:HG3	1:B:184:MET:SD	2.51	0.50
1:B:79:ASN:O	1:B:131:SER:HA	2.11	0.50
1:A:514:ARG:HD3	6:A:965:HOH:O	2.11	0.50
1:B:69:PHE:CE2	1:B:121:ASP:HB2	2.47	0.49
1:A:78:ARG:HG2	1:A:78:ARG:HH11	1.77	0.49
1:B:70:VAL:CG2	1:B:121:ASP:HB3	2.36	0.49
1:B:167:LYS:HB3	1:B:200:ILE:CD1	2.43	0.49
1:A:294:GLN:H	1:A:294:GLN:CD	2.21	0.49
1:A:378:THR:O	1:A:426:HIS:HB3	2.12	0.49
1:B:253:MET:HE3	1:B:364:PRO:HG3	1.94	0.49
1:B:619:LEU:H	1:B:619:LEU:CD1	2.25	0.49
1:A:401:HIS:O	1:A:405:MET:HG2	2.13	0.48
1:B:484:ARG:HD2	1:B:484:ARG:N	2.28	0.48
1:B:643:THR:O	1:B:647:ILE:HG13	2.13	0.48
1:A:423:ALA:HA	1:A:481:LYS:HB2	1.95	0.48
1:B:418:SER:HA	1:B:422:GLU:HB3	1.96	0.48
1:A:80:ILE:HG23	1:A:109:GLY:CA	2.44	0.48
1:B:119:LEU:N	1:B:119:LEU:HD22	2.29	0.48
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.96	0.48
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.94	0.48
1:A:263:MET:HE2	1:A:323:TYR:CE1	2.49	0.48
1:A:606:GLN:HA	1:A:609:LEU:HD12	1.96	0.47
1:B:96:ASN:O	1:B:100:LYS:HG3	2.14	0.47
1:B:143:GLY:HA2	1:B:183:ALA:HB3	1.96	0.47
1:A:291:LYS:HE3	1:A:293:ASN:O	2.14	0.47
1:A:177:THR:HB	1:A:634:ARG:CB	2.44	0.47
1:A:297:GLU:C	1:A:298:ARG:HG3	2.39	0.47
1:B:385:VAL:O	1:B:389:LEU:HG	2.14	0.47
1:A:578:GLU:O	1:A:581:ARG:HB3	2.13	0.47
1:B:599:GLN:N	1:B:599:GLN:CD	2.72	0.47
1:B:619:LEU:N	1:B:619:LEU:CD1	2.78	0.47
1:A:298:ARG:NH2	4:A:703:NAP:H51N	2.30	0.47
1:A:561:LEU:N	1:A:561:LEU:HD12	2.30	0.46
1:B:107:MET:HE1	1:B:227:VAL:CG1	2.45	0.46
1:B:126:PRO:HG3	1:B:165:GLY:C	2.40	0.46
1:B:264:GLY:O	1:B:265:ARG:C	2.57	0.46
1:B:592:ASN:HB3	1:B:608:LEU:HD13	1.97	0.46
1:A:88:THR:HG22	1:A:88:THR:O	2.15	0.46
1:A:581:ARG:HE	1:A:581:ARG:HA	1.80	0.46
1:A:83:PHE:HA	1:A:112:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:HB	2:A:701:FMN:O1P	2.15	0.46
1:A:288:ALA:O	1:A:303:LEU:HA	2.15	0.46
1:B:125:LEU:HD23	1:B:166:VAL:HG13	1.96	0.46
1:B:125:LEU:N	1:B:126:PRO:CD	2.79	0.46
1:A:80:ILE:HG23	1:A:109:GLY:HA3	1.98	0.46
1:B:258:VAL:HG13	1:B:365:THR:HA	1.98	0.46
1:A:140:TYR:O	1:A:141:GLY:O	2.34	0.46
1:B:180:HIS:HB3	1:B:183:ALA:HB2	1.98	0.46
1:A:298:ARG:HD3	6:A:808:HOH:O	2.16	0.45
1:A:306:ASP:OD1	1:A:308:SER:HB2	2.16	0.45
1:A:298:ARG:HH21	4:A:703:NAP:H51N	1.80	0.45
1:A:107:MET:HE2	1:A:233:VAL:HG21	1.99	0.45
1:B:649:ALA:HB2	1:B:659:ALA:HB2	1.98	0.45
1:A:533:PRO:HG3	1:A:636:MET:HG3	1.98	0.45
1:B:376:ASP:OD2	1:B:379:ASN:ND2	2.49	0.45
1:B:665:LYS:HE2	1:B:669:LYS:HE3	1.99	0.45
1:A:68:SER:HA	6:A:943:HOH:O	2.17	0.45
1:A:652:GLY:N	1:A:653:PRO:HA	2.32	0.45
1:B:76:THR:CG2	1:B:78:ARG:HE	2.29	0.45
1:B:310:SER:O	1:B:311:LYS:HB2	2.17	0.45
1:B:114:PRO:HG2	1:B:148:ASN:O	2.17	0.45
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.99	0.45
1:A:125:LEU:N	1:A:126:PRO:CD	2.80	0.44
1:B:569:SER:HB2	1:B:576:ARG:NH1	2.32	0.44
1:B:660:VAL:O	1:B:664:LYS:HD3	2.17	0.44
1:A:634:ARG:O	1:A:638:LYS:CG	2.65	0.44
1:B:130:LYS:HA	1:B:231:PHE:CD1	2.52	0.44
1:B:263:MET:HE2	1:B:323:TYR:CE1	2.51	0.44
1:A:283:LEU:N	1:A:283:LEU:HD12	2.33	0.44
1:B:94:PHE:HB3	1:B:216:PHE:CE1	2.52	0.44
1:A:418:SER:HA	1:A:422:GLU:HB3	2.00	0.44
1:B:475:ALA:HA	1:B:491:THR:HB	1.99	0.44
1:B:613:ARG:HG2	1:B:613:ARG:HH11	1.82	0.44
1:A:84:TYR:CZ	1:A:92:GLU:HG3	2.52	0.44
1:B:378:THR:O	1:B:426:HIS:HB3	2.17	0.44
1:A:335:GLY:HA3	1:A:342:LEU:HD21	2.00	0.44
1:B:361:PHE:O	1:B:362:PRO:C	2.60	0.44
1:B:537:ILE:O	1:B:537:ILE:HG13	2.17	0.44
1:B:69:PHE:O	1:B:73:MET:HG3	2.17	0.44
1:B:93:GLU:OE1	1:B:93:GLU:HA	2.17	0.44
1:A:256:ALA:HA	1:A:267:LYS:HZ3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:HIS:HE1	1:B:304:GLU:OE1	2.01	0.43
1:B:389:LEU:HD21	1:B:447:LEU:HD12	1.99	0.43
1:B:626:HIS:CD2	1:B:671:ARG:HG2	2.53	0.43
1:A:145:PRO:HG2	1:A:153:TYR:CG	2.53	0.43
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.99	0.43
1:A:78:ARG:NH1	1:A:108:ARG:HD3	2.32	0.43
1:B:74:LYS:HG3	1:B:128:ILE:HD11	2.01	0.43
1:A:217:ILE:HD11	1:A:383:THR:HG21	2.00	0.43
1:A:366:THR:HG23	6:A:836:HOH:O	2.18	0.43
1:A:467:ASN:HB2	5:A:704:PO4:P	2.59	0.43
1:B:352:ASP:C	1:B:354:GLU:H	2.26	0.43
1:B:540:PHE:HA	1:B:543:PHE:HB2	2.00	0.43
1:B:69:PHE:CD1	1:B:69:PHE:C	2.97	0.42
1:B:76:THR:HG21	1:B:78:ARG:HE	1.83	0.42
1:A:617:TRP:CD1	1:A:651:PHE:HB3	2.54	0.42
1:A:304:GLU:HG2	1:A:470:HIS:CD2	2.54	0.42
1:B:79:ASN:ND2	1:B:80:ILE:HG13	2.34	0.42
1:B:214:GLU:CD	1:B:413:LYS:HE3	2.44	0.42
1:B:323:TYR:CE1	1:B:453:ALA:HB2	2.54	0.42
1:B:76:THR:HG21	1:B:352:ASP:OD2	2.20	0.42
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.84	0.42
1:B:140:TYR:O	1:B:144:ASP:HB2	2.19	0.42
1:A:119:LEU:N	1:A:119:LEU:HD22	2.34	0.42
1:B:167:LYS:HD2	1:B:200:ILE:HD11	2.01	0.42
1:A:78:ARG:HH11	1:A:108:ARG:HG2	1.85	0.42
1:A:337:ILE:HB	1:B:600:ALA:HB1	2.02	0.42
1:B:79:ASN:ND2	1:B:107:MET:SD	2.92	0.42
1:B:629:VAL:HB	1:B:674:LEU:CD2	2.47	0.42
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.94	0.41
1:B:89:GLY:O	1:B:93:GLU:HB2	2.20	0.41
1:B:541:MET:HE2	1:B:575:TYR:CG	2.55	0.41
1:B:447:LEU:HA	6:B:807:HOH:O	2.19	0.41
1:B:610:LYS:HD2	1:B:610:LYS:HA	1.89	0.41
1:A:653:PRO:O	1:A:654:MET:HB3	2.21	0.41
1:B:152:PHE:CE1	1:B:156:LEU:HD21	2.55	0.41
1:B:521:PRO:HG3	1:B:626:HIS:ND1	2.35	0.41
1:B:294:GLN:H	1:B:294:GLN:CD	2.28	0.41
1:A:441:ILE:HG23	1:A:442:ASP:N	2.35	0.41
1:B:146:THR:O	1:B:147:ASP:C	2.64	0.41
1:A:633:ALA:CB	1:A:678:SER:HA	2.41	0.41
1:A:599:GLN:HG2	1:A:601:HIS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:HIS:O	1:A:659:ALA:HB3	2.20	0.41
1:B:84:TYR:CG	1:B:92:GLU:HA	2.56	0.41
1:B:64:VAL:HG23	1:B:64:VAL:O	2.21	0.41
1:A:100:LYS:HE3	1:A:244:GLN:OE1	2.20	0.40
1:A:642:ASN:HA	1:A:645:TYR:CD2	2.56	0.40
1:B:427:ILE:O	1:B:431:LEU:HG	2.21	0.40
3:A:702:FAD:H1'1	3:A:702:FAD:H9	1.83	0.40
1:B:338:LEU:CD2	1:B:439:PRO:HD2	2.51	0.40
1:B:418:SER:HA	1:B:422:GLU:CB	2.52	0.40
1:B:547:ARG:O	1:B:551:ARG:HG3	2.21	0.40
1:A:173:LEU:HD23	1:A:212:LEU:HD21	2.04	0.40
1:B:194:GLN:C	1:B:195:LEU:HD12	2.46	0.40
1:A:317:GLY:HA3	1:A:518:PHE:O	2.22	0.40
1:B:80:ILE:HG12	1:B:132:LEU:HB3	2.04	0.40
1:B:395:GLU:HB3	1:B:436:SER:OG	2.22	0.40
1:A:67:SER:O	1:A:68:SER:C	2.64	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	599/622 (96%)	577 (96%)	20 (3%)	2 (0%)	36	55
1	B	598/622 (96%)	555 (93%)	43 (7%)	0	100	100
All	All	1197/1244 (96%)	1132 (95%)	63 (5%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	GLY
1	A	635	ASN

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	516/530 (97%)	503 (98%)	13 (2%)	42	69
1	B	508/530 (96%)	502 (99%)	6 (1%)	63	83
All	All	1024/1060 (97%)	1005 (98%)	19 (2%)	50	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	151	ASP
1	A	221	GLU
1	A	294	GLN
1	A	479	GLU
1	A	484	ARG
1	A	487	LYS
1	A	573	TYR
1	A	598	GLU
1	A	614	GLU
1	A	635	ASN
1	A	638	LYS
1	A	674	LEU
1	B	324	PRO
1	B	330	LEU
1	B	396	PRO
1	B	484	ARG
1	B	581	ARG
1	B	638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	294	GLN
1	A	399	GLN

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Mol	Chain	Res	Type
1	A	452	GLN
1	A	467	ASN
1	A	470	HIS
1	A	486	ASN
1	A	599	GLN
1	B	194	GLN
1	B	280	ASN
1	B	302	HIS
1	B	465	HIS
1	B	467	ASN
1	B	470	HIS
1	B	545	GLN
1	B	590	GLN
1	B	592	ASN
1	B	635	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 oligosaccharides 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
5	PO4	B	704	-	4,4,4	1.67	0	6,6,6	0.47	0
4	NAP	B	703	-	42,43,52	1.43	7 (16%)	62,67,80	1.77	14 (22%)
4	NAP	A	703	-	42,43,52	1.44	7 (16%)	62,67,80	1.75	12 (19%)
5	PO4	A	704	-	4,4,4	1.69	0	6,6,6	0.46	0
2	FMN	A	701	-	33,33,33	2.65	14 (42%)	48,50,50	1.63	13 (27%)
2	FMN	B	701	-	33,33,33	2.67	14 (42%)	48,50,50	1.64	12 (25%)
3	FAD	B	702	-	58,58,58	2.30	12 (20%)	85,89,89	2.00	18 (21%)
3	FAD	A	702	-	58,58,58	2.31	13 (22%)	85,89,89	1.95	16 (18%)

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
4	NAP	B	703	-	-	5/27/59/67	0/4/4/5
4	NAP	A	703	-	-	5/27/59/67	0/4/4/5
2	FMN	A	701	-	-	0/18/18/18	0/3/3/3
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3
3	FAD	B	702	-	-	1/34/50/50	0/6/6/6
3	FAD	A	702	-	-	0/34/50/50	0/6/6/6

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C8A-N7A	8.60	1.48	1.31
3	B	702	FAD	C8A-N7A	8.59	1.48	1.31
2	B	701	FMN	C8M-C8	-6.78	1.38	1.51
2	A	701	FMN	C8M-C8	-6.62	1.38	1.51
3	A	702	FAD	C8M-C8	-6.18	1.39	1.51
3	A	702	FAD	C8A-N9A	6.18	1.48	1.37
3	B	702	FAD	C8M-C8	-6.16	1.39	1.51
3	B	702	FAD	C8A-N9A	6.12	1.48	1.37
3	A	702	FAD	C7M-C7	-6.09	1.39	1.51
3	B	702	FAD	C7M-C7	-6.08	1.39	1.51
2	A	701	FMN	C4A-N5	5.34	1.42	1.30
2	B	701	FMN	C4A-N5	5.30	1.42	1.30
2	B	701	FMN	C10-N10	5.22	1.48	1.37
2	B	701	FMN	C9-C9A	5.11	1.47	1.39
2	A	701	FMN	C10-N10	4.91	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FMN	C9A-C5A	4.62	1.48	1.41
2	A	701	FMN	C9-C9A	4.62	1.47	1.39
2	A	701	FMN	C9A-N10	4.33	1.48	1.41
2	B	701	FMN	C9A-N10	4.25	1.48	1.41
2	A	701	FMN	C8-C7	4.05	1.50	1.40
2	B	701	FMN	C9A-C5A	4.02	1.47	1.41
2	B	701	FMN	C8-C7	3.98	1.50	1.40
3	A	702	FAD	C9A-N10	-3.77	1.34	1.41
3	B	702	FAD	C9A-N10	-3.69	1.34	1.41
4	B	703	NAP	C2A-N3A	3.67	1.40	1.33
4	A	703	NAP	C2A-N3A	3.67	1.40	1.33
3	B	702	FAD	C2A-N3A	3.66	1.40	1.33
4	A	703	NAP	C2A-N1A	3.64	1.40	1.33
3	A	702	FAD	C2A-N1A	3.61	1.40	1.33
3	A	702	FAD	C2A-N3A	3.60	1.40	1.33
4	B	703	NAP	C2A-N1A	3.59	1.40	1.33
3	A	702	FAD	C10-N1	3.54	1.40	1.33
3	B	702	FAD	C10-N1	3.53	1.40	1.33
3	B	702	FAD	C2A-N1A	3.50	1.40	1.33
2	B	701	FMN	C10-N1	3.42	1.40	1.33
2	A	701	FMN	C6-C5A	3.36	1.45	1.40
4	A	703	NAP	C5A-N7A	-3.08	1.33	1.39
4	A	703	NAP	C5A-C4A	-3.07	1.33	1.39
2	B	701	FMN	C6-C5A	3.07	1.44	1.40
2	A	701	FMN	C10-N1	3.07	1.39	1.33
4	B	703	NAP	C5A-C4A	-3.05	1.33	1.39
3	B	702	FAD	C5A-N7A	-3.03	1.33	1.39
3	A	702	FAD	C5A-N7A	-3.03	1.33	1.39
4	B	703	NAP	C5A-N7A	-3.00	1.33	1.39
3	B	702	FAD	C5A-C4A	-2.95	1.33	1.39
3	A	702	FAD	C5A-C4A	-2.94	1.33	1.39
3	B	702	FAD	C5X-N5	-2.69	1.34	1.39
3	A	702	FAD	C5X-N5	-2.68	1.34	1.39
3	B	702	FAD	C5A-C6A	-2.66	1.33	1.41
3	A	702	FAD	C5A-C6A	-2.65	1.33	1.41
4	A	703	NAP	C5A-C6A	-2.63	1.33	1.41
4	B	703	NAP	C5A-C6A	-2.61	1.33	1.41
2	B	701	FMN	O2'-C2'	2.49	1.48	1.43
4	A	703	NAP	C8A-N9A	-2.46	1.33	1.37
4	B	703	NAP	C8A-N9A	-2.42	1.33	1.37
2	B	701	FMN	C4'-C3'	2.40	1.57	1.53
2	A	701	FMN	O2'-C2'	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FMN	C7M-C7	2.23	1.55	1.51
2	B	701	FMN	C7M-C7	2.21	1.55	1.51
2	A	701	FMN	C6-C7	2.12	1.42	1.39
2	A	701	FMN	C1'-C2'	2.12	1.55	1.52
2	B	701	FMN	C1'-C2'	2.07	1.55	1.52
2	B	701	FMN	C6-C7	2.04	1.42	1.39
4	A	703	NAP	C4A-N9A	-2.02	1.33	1.37
4	B	703	NAP	C4A-N9A	-2.01	1.33	1.37
3	A	702	FAD	C4A-N9A	-2.00	1.33	1.37
2	A	701	FMN	C4'-C3'	2.00	1.56	1.53

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N9A-C8A-N7A	-9.76	100.09	113.94
3	B	702	FAD	N9A-C8A-N7A	-9.64	100.26	113.94
3	B	702	FAD	N3A-C2A-N1A	-7.53	117.19	128.58
3	A	702	FAD	N3A-C2A-N1A	-7.47	117.27	128.58
4	A	703	NAP	N3A-C2A-N1A	-7.08	117.86	128.58
4	B	703	NAP	N3A-C2A-N1A	-7.03	117.93	128.58
3	B	702	FAD	C5A-C4A-N3A	-4.74	120.19	126.72
4	A	703	NAP	N9A-C8A-N7A	-4.43	107.66	113.94
4	B	703	NAP	N9A-C8A-N7A	-4.42	107.66	113.94
3	A	702	FAD	C5A-C4A-N3A	-4.34	120.74	126.72
4	B	703	NAP	C5A-C4A-N3A	-4.26	120.86	126.72
4	A	703	NAP	C5A-C4A-N3A	-4.23	120.89	126.72
3	B	702	FAD	C5A-C4A-N9A	4.08	110.26	105.81
2	A	701	FMN	O4'-C4'-C3'	-3.99	99.92	109.25
2	B	701	FMN	C9A-C5A-N5	3.92	126.62	122.45
2	A	701	FMN	C9A-C5A-N5	3.86	126.55	122.45
3	B	702	FAD	C2A-N3A-C4A	3.72	120.91	111.83
2	B	701	FMN	O4'-C4'-C3'	-3.60	100.83	109.25
3	A	702	FAD	C2A-N3A-C4A	3.54	120.48	111.83
3	A	702	FAD	C5A-C4A-N9A	3.50	109.62	105.81
3	B	702	FAD	C5A-N7A-C8A	3.42	108.82	103.45
3	A	702	FAD	C5A-N7A-C8A	3.36	108.73	103.45
4	B	703	NAP	C2A-N3A-C4A	3.27	119.83	111.83
4	A	703	NAP	C2A-N3A-C4A	3.26	119.79	111.83
4	B	703	NAP	C5A-N7A-C8A	3.17	108.44	103.45
4	A	703	NAP	C5A-N7A-C8A	3.06	108.25	103.45
3	A	702	FAD	C4-N3-C2	-3.00	120.31	125.64
3	B	702	FAD	C5A-C6A-N6A	-3.00	115.87	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	FAD	C4-N3-C2	-2.99	120.33	125.64
2	B	701	FMN	C5A-C9A-N10	-2.94	115.31	117.97
2	B	701	FMN	C4'-C3'-C2'	-2.94	108.68	113.57
4	A	703	NAP	C5A-C6A-N6A	-2.88	116.15	123.29
3	B	702	FAD	C4A-N9A-C8A	2.87	108.75	105.74
3	A	702	FAD	C5A-C6A-N6A	-2.85	116.23	123.29
2	B	701	FMN	O4-C4-N3	-2.82	114.82	120.11
3	B	702	FAD	C2B-C3B-C4B	-2.78	97.23	102.61
3	A	702	FAD	C10-C4X-N5	-2.75	119.20	124.81
3	B	702	FAD	C10-C4X-N5	-2.72	119.25	124.81
2	A	701	FMN	C4'-C3'-C2'	-2.69	109.09	113.57
2	A	701	FMN	C5A-C9A-N10	-2.66	115.56	117.97
2	A	701	FMN	O4-C4-N3	-2.65	115.12	120.11
2	B	701	FMN	O3P-P-O5'	-2.64	99.79	106.67
2	A	701	FMN	C8M-C8-C7	2.61	126.10	120.76
2	A	701	FMN	C5A-N5-C4A	-2.60	113.88	118.09
3	B	702	FAD	C4X-C4-N3	2.60	119.88	113.25
4	B	703	NAP	C4A-C5A-N7A	-2.60	107.61	110.58
4	A	703	NAP	C6A-C5A-C4A	2.57	120.69	117.18
4	B	703	NAP	C5A-C6A-N6A	-2.57	116.93	123.29
4	B	703	NAP	C6A-C5A-C4A	2.56	120.68	117.18
3	A	702	FAD	C4X-C4-N3	2.53	119.70	113.25
2	B	701	FMN	C8M-C8-C7	2.52	125.90	120.76
3	A	702	FAD	C4A-N9A-C8A	2.49	108.36	105.74
4	A	703	NAP	C4A-N9A-C8A	2.49	108.36	105.74
3	A	702	FAD	C2B-C3B-C4B	-2.43	97.91	102.61
2	A	701	FMN	O4'-C4'-C5'	-2.43	104.64	109.99
2	A	701	FMN	C8M-C8-C9	-2.42	115.31	119.57
4	B	703	NAP	C4A-N9A-C8A	2.36	108.22	105.74
4	B	703	NAP	C3B-C2B-C1B	-2.36	98.29	102.81
2	B	701	FMN	C9-C9A-N10	2.35	125.02	121.85
4	A	703	NAP	C4A-C5A-N7A	-2.35	107.90	110.58
3	B	702	FAD	C6A-C5A-C4A	2.33	120.36	117.18
2	B	701	FMN	O2P-P-O1P	2.33	119.90	110.83
2	B	701	FMN	C5A-N5-C4A	-2.31	114.35	118.09
3	A	702	FAD	O4-C4-C4X	-2.29	120.49	126.53
4	B	703	NAP	N3A-C4A-N9A	2.29	131.06	127.17
2	A	701	FMN	O2P-P-O1P	2.29	119.74	110.83
3	A	702	FAD	C9A-C5X-N5	-2.25	120.06	122.45
4	A	703	NAP	C3B-C2B-C1B	-2.25	98.50	102.81
3	B	702	FAD	C4X-C10-N10	2.24	119.68	116.48
4	A	703	NAP	N3A-C4A-N9A	2.23	130.96	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	FAD	O4-C4-C4X	-2.23	120.66	126.53
2	A	701	FMN	O3P-P-O5'	-2.21	100.92	106.67
2	B	701	FMN	C7M-C7-C6	-2.19	115.71	119.57
2	B	701	FMN	C8M-C8-C9	-2.18	115.74	119.57
3	B	702	FAD	C5'-C4'-C3'	-2.17	108.12	112.22
3	A	702	FAD	C6A-C5A-C4A	2.17	120.14	117.18
3	B	702	FAD	C9A-C5X-N5	-2.16	120.16	122.45
2	A	701	FMN	C7M-C7-C6	-2.15	115.79	119.57
4	A	703	NAP	O4B-C1B-C2B	-2.09	102.99	106.59
4	B	703	NAP	C5A-C4A-N9A	2.06	108.06	105.81
3	A	702	FAD	C4X-C10-N10	2.05	119.42	116.48
2	A	701	FMN	C9-C9A-N10	2.04	124.60	121.85
3	B	702	FAD	C5A-C6A-N1A	2.03	122.66	117.51
4	B	703	NAP	C2D-C3D-C4D	-2.02	98.70	102.61
4	B	703	NAP	O4B-C1B-N9A	2.02	111.97	108.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

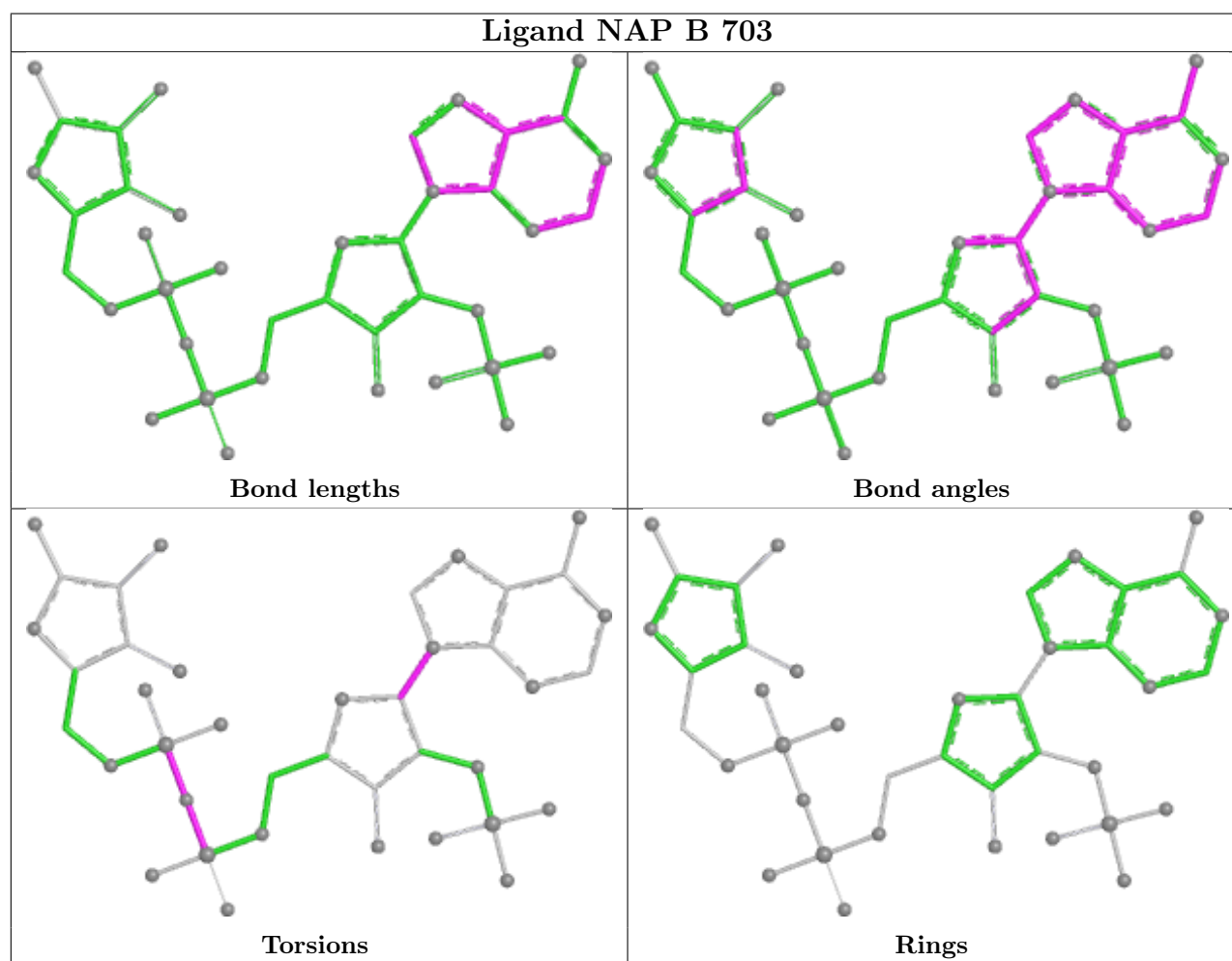
Mol	Chain	Res	Type	Atoms
4	A	703	NAP	C2B-C1B-N9A-C8A
4	A	703	NAP	C5D-O5D-PN-O3
4	A	703	NAP	C5D-O5D-PN-O1N
4	A	703	NAP	C2B-C1B-N9A-C4A
4	B	703	NAP	C2B-C1B-N9A-C8A
4	B	703	NAP	C2B-C1B-N9A-C4A
4	A	703	NAP	C5D-O5D-PN-O2N
4	B	703	NAP	PA-O3-PN-O1N
3	B	702	FAD	PA-O3P-P-O2P
4	B	703	NAP	O4B-C1B-N9A-C8A
4	B	703	NAP	PN-O3-PA-O2A

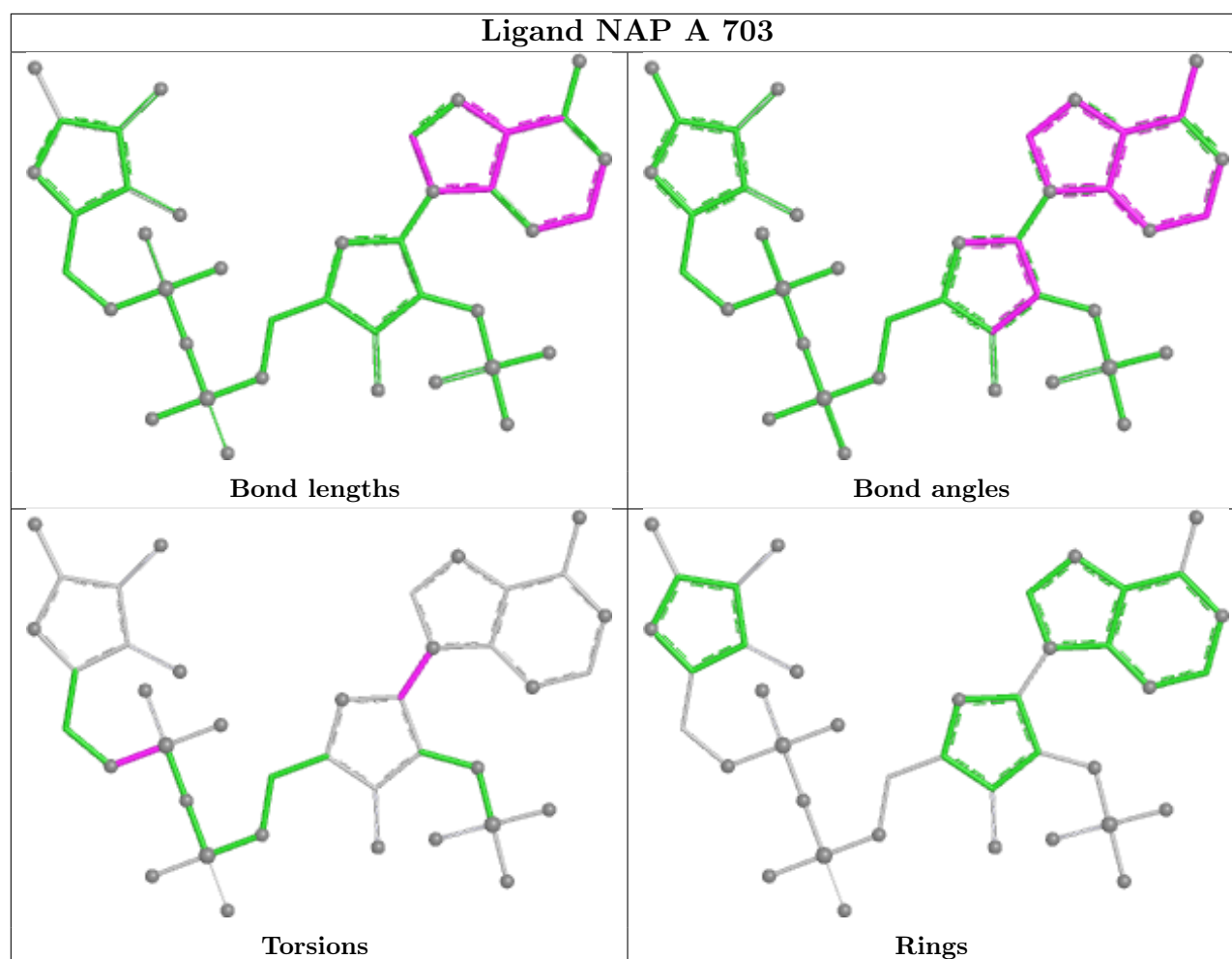
There are no ring outliers.

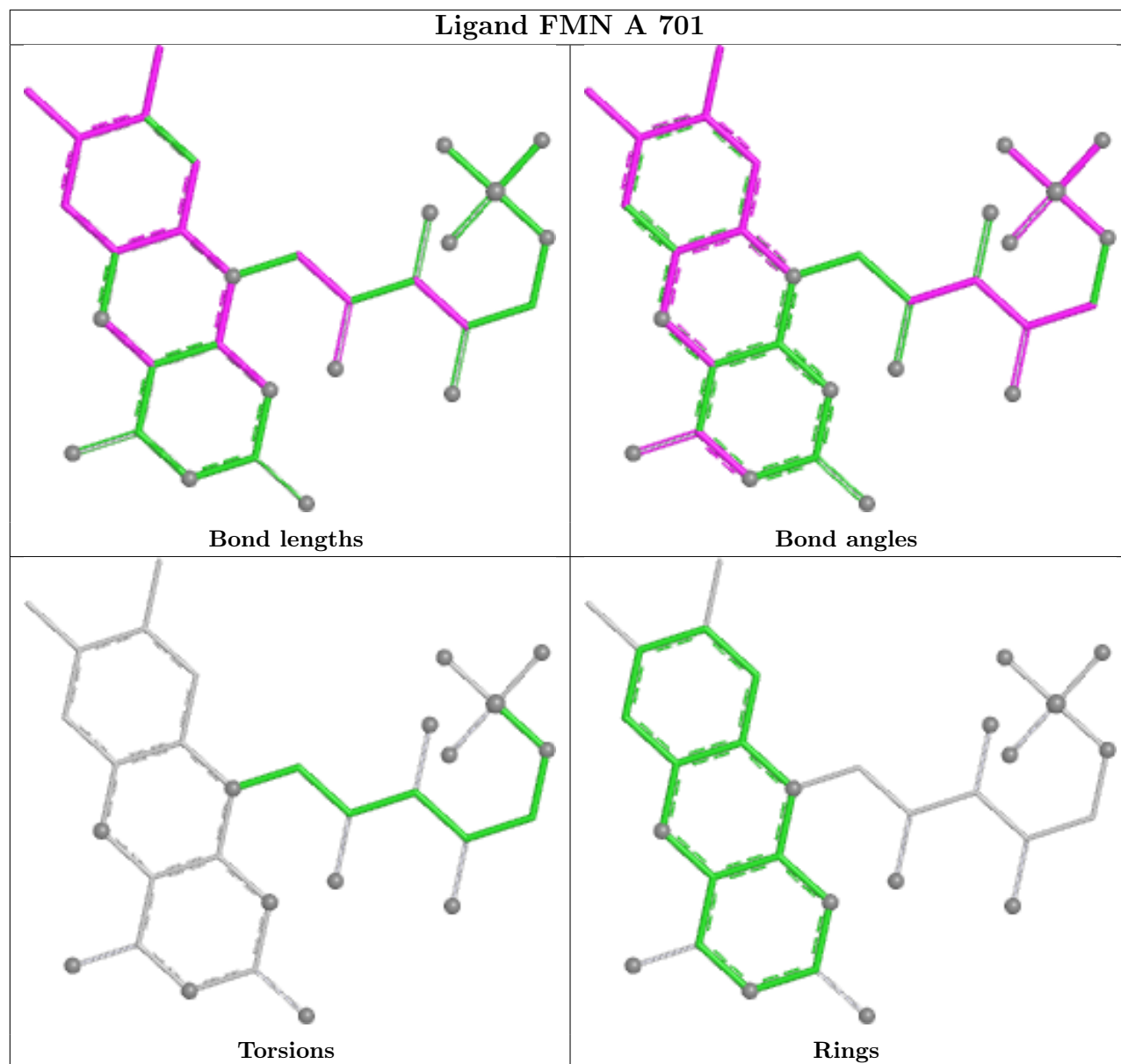
4 monomers are involved in 6 short contacts:

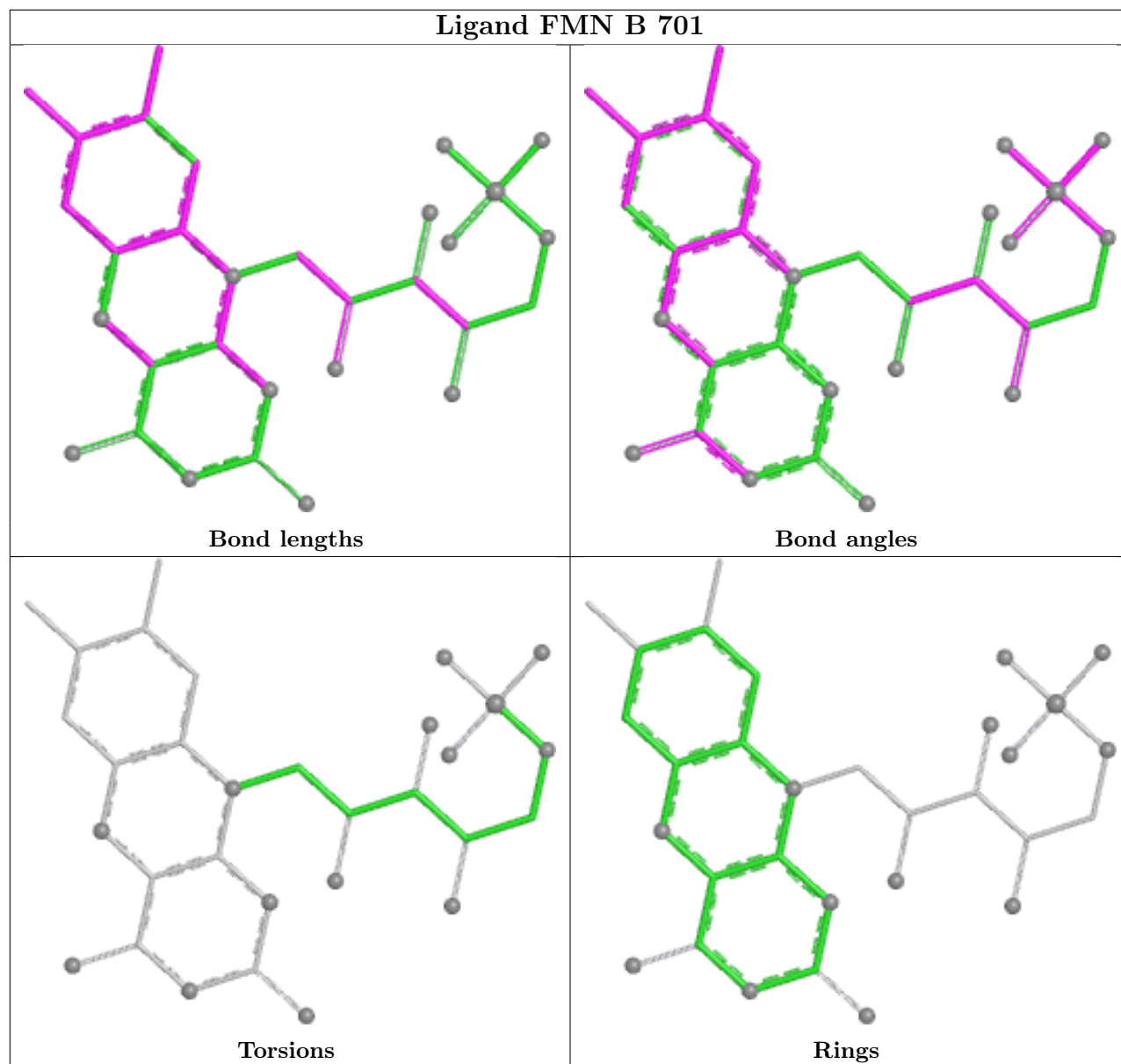
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	NAP	3	0
5	A	704	PO4	1	0
2	A	701	FMN	1	0
3	A	702	FAD	1	0

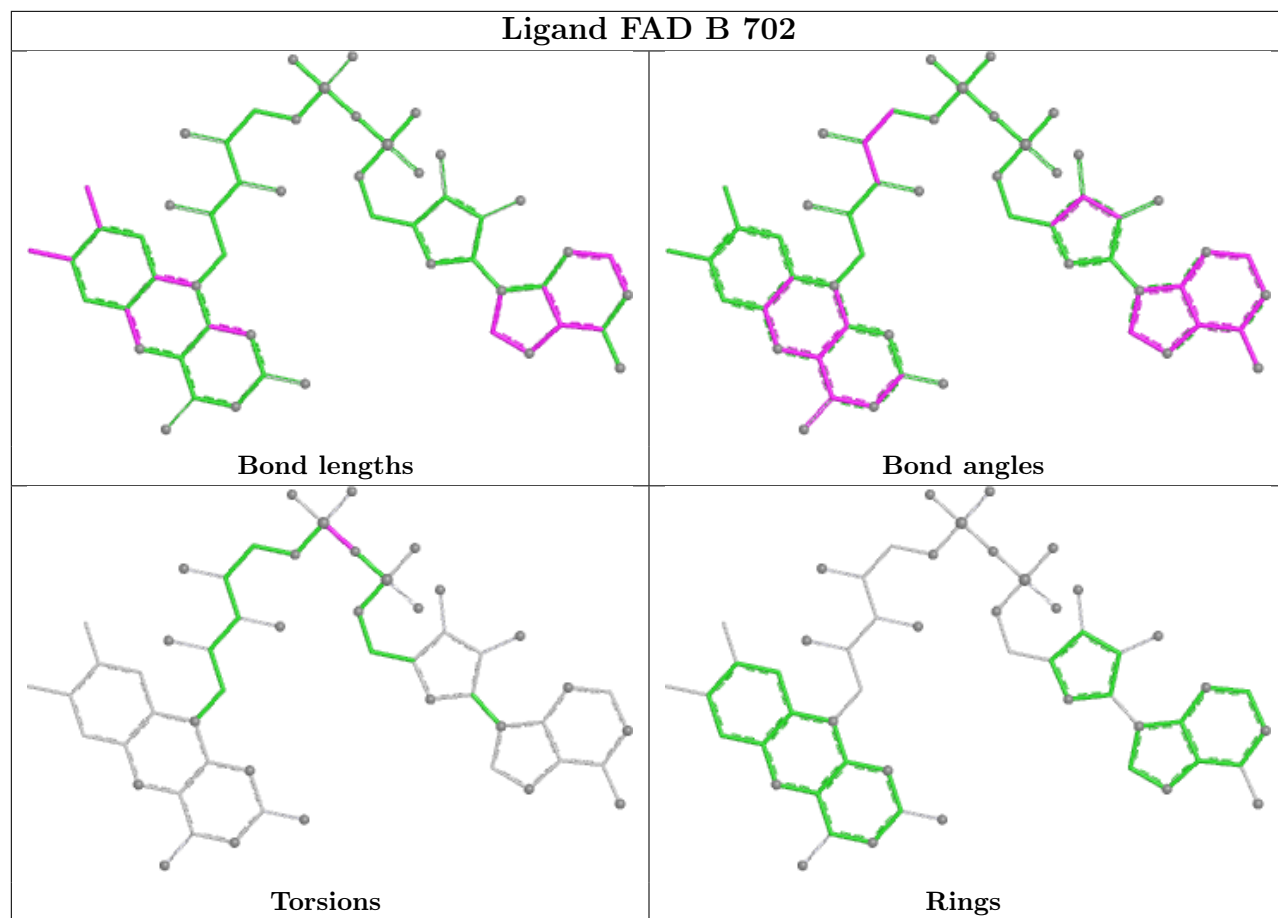
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

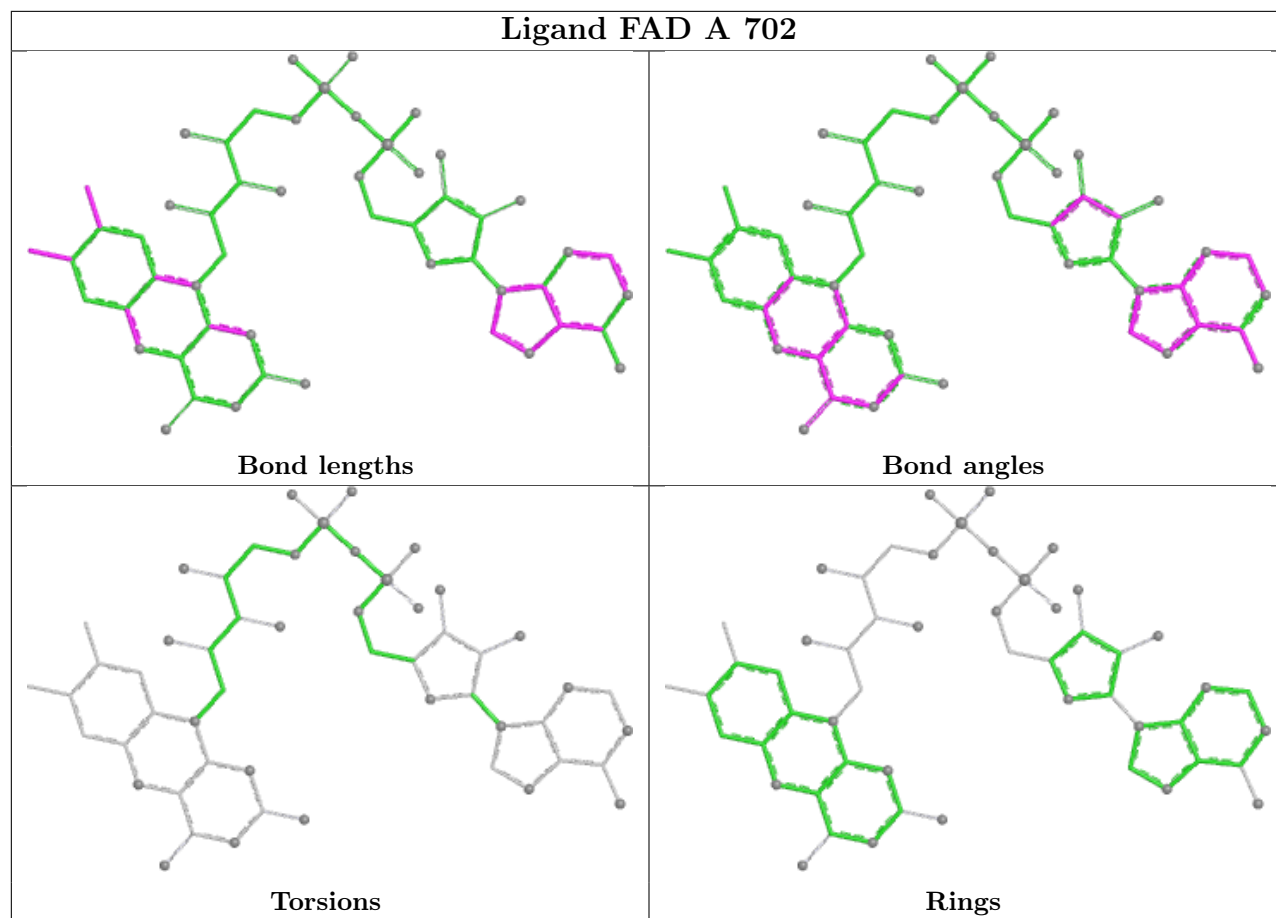












5.7 Other polymers [i](#)

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%)	-0.15	8 (1%) 75 71	22, 39, 59, 75	0
1	B	606/622 (97%)	0.31	27 (4%) 38 33	19, 49, 92, 100	0
All	All	1215/1244 (97%)	0.08	35 (2%) 53 49	19, 43, 88, 100	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	633	ALA	3.9
1	A	633	ALA	3.7
1	B	160	ASP	3.7
1	B	63	PRO	3.4
1	B	236	THR	3.2
1	A	678	SER	3.1
1	B	179	GLU	3.1
1	B	161	VAL	3.0
1	B	242	ILE	2.9
1	B	162	ASP	2.9
1	A	240	SER	2.8
1	B	235	ALA	2.8
1	B	500	ALA	2.8
1	B	255	VAL	2.8
1	B	67	SER	2.7
1	A	634	ARG	2.7
1	B	159	THR	2.7
1	A	229	GLU	2.6
1	B	163	LEU	2.5
1	B	192	LEU	2.5
1	B	678	SER	2.4
1	B	119	LEU	2.4
1	A	141	GLY	2.4
1	B	188	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	112	ALA	2.2
1	A	506	ARG	2.2
1	B	102	ALA	2.2
1	B	252	ASP	2.2
1	B	152	PHE	2.2
1	B	103	HIS	2.1
1	B	156	LEU	2.1
1	B	656	HIS	2.1
1	A	505	GLY	2.0
1	B	158	GLU	2.0
1	B	64	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

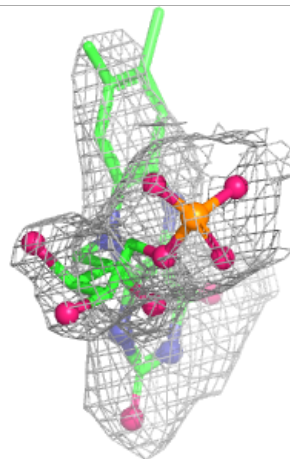
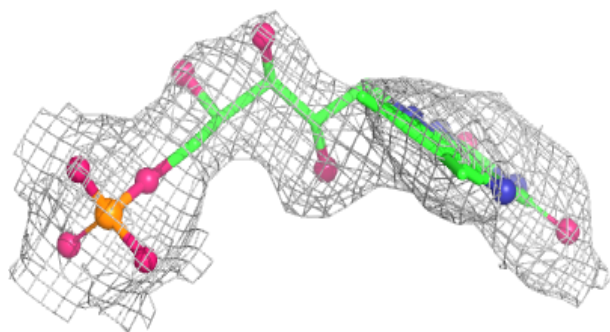
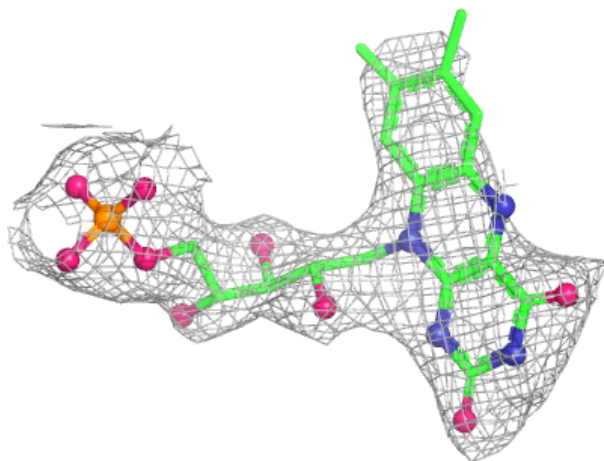
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.46	0.19	160,160,160,161	0
5	PO4	B	704	5/5	0.80	0.12	96,96,97,97	0
2	FMN	B	701	31/31	0.91	0.12	65,83,86,86	0
4	NAP	B	703	40/48	0.96	0.09	31,37,78,85	0
2	FMN	A	701	31/31	0.96	0.08	31,44,49,51	0
4	NAP	A	703	40/48	0.96	0.08	27,34,80,86	0
3	FAD	A	702	53/53	0.97	0.07	24,28,44,46	0
3	FAD	B	702	53/53	0.98	0.06	16,23,35,36	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.

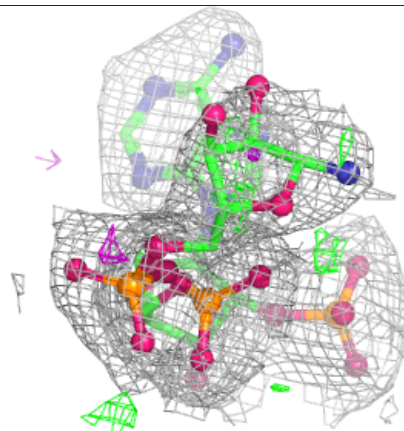
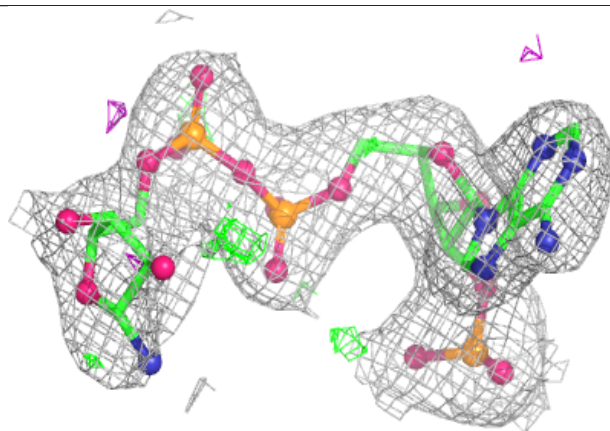
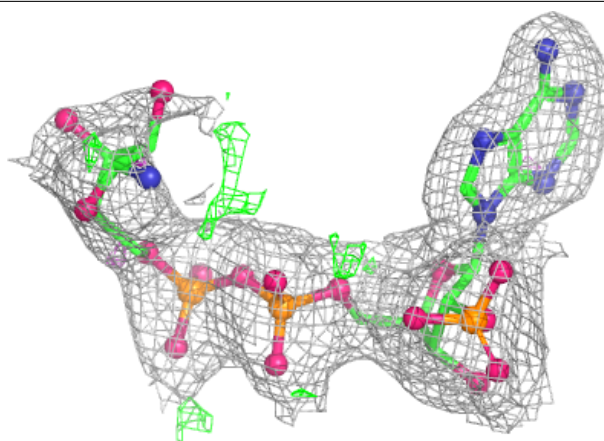
Electron density around FMN B 701:

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



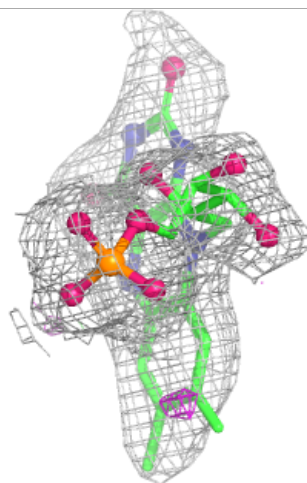
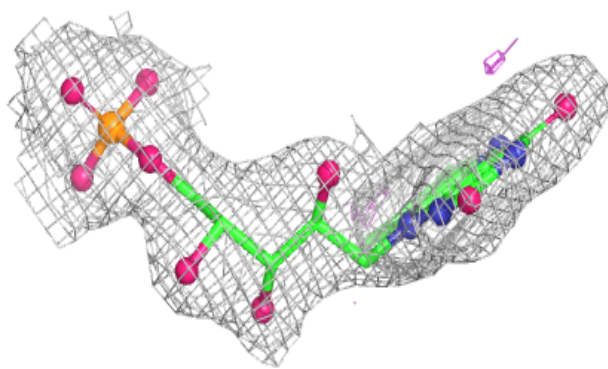
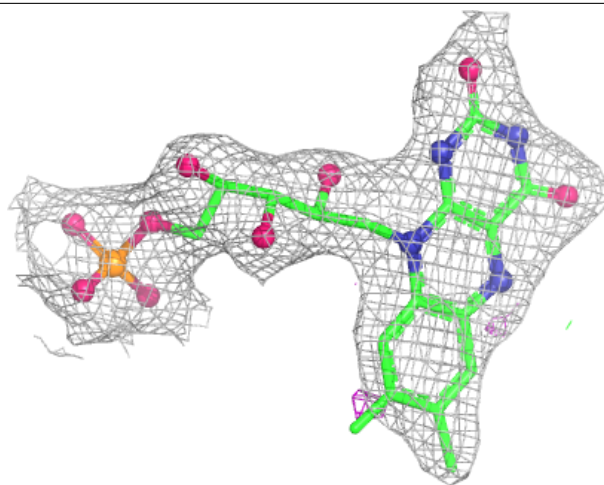
Electron density around NAP B 703:

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



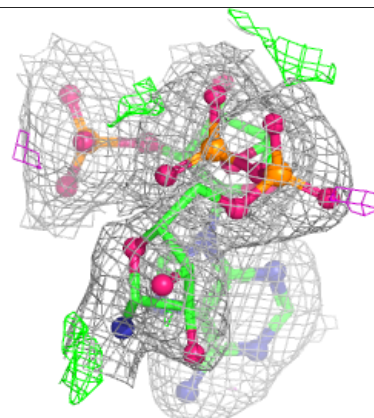
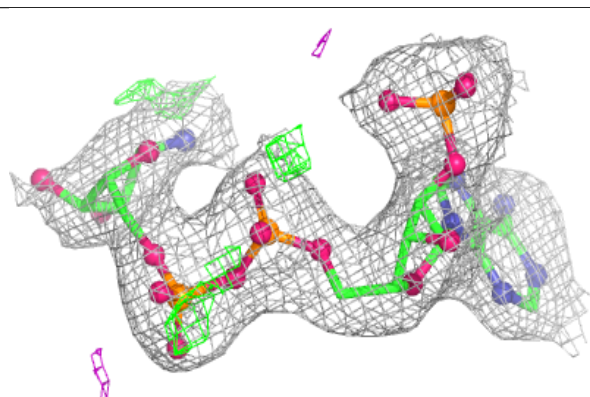
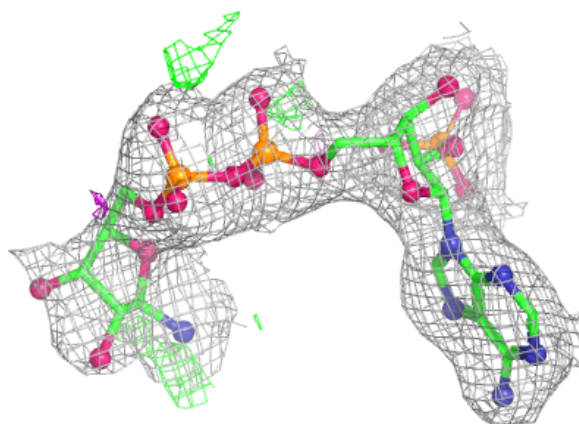
Electron density around FMN A 701:

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

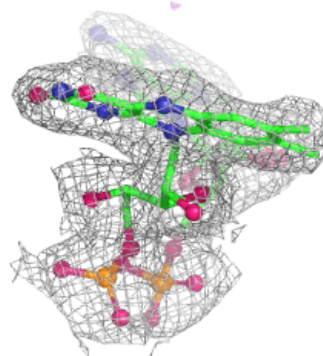
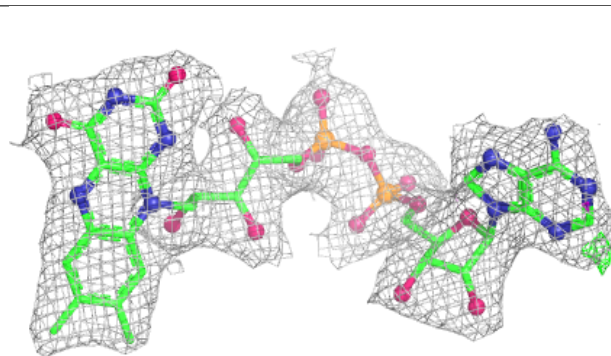
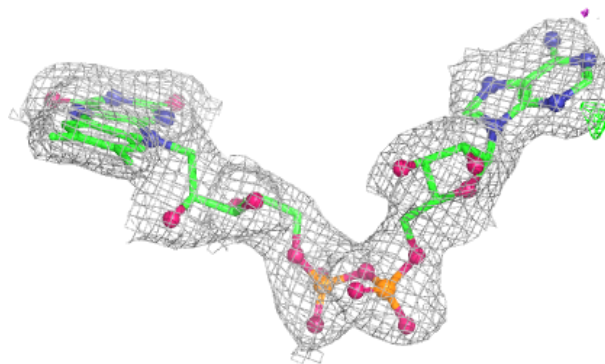


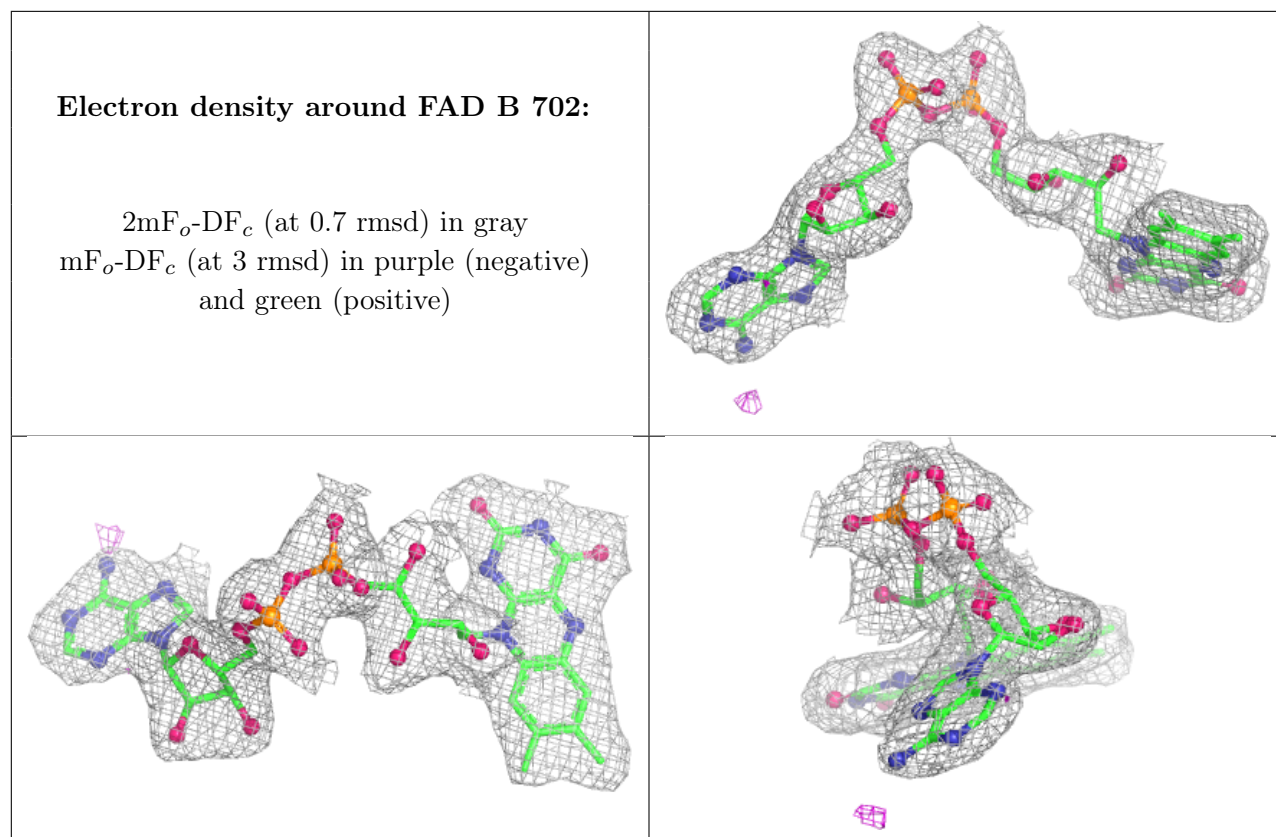
Electron density around NAP A 703:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.