



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:19 PM UTC

PDB ID : 4Y9U / pdb_00004y9u
Title : rat CYPOR mutant - G143del
Authors : Xia, C.; Kim, J.J.P.
Deposited on : 2015-02-17
Resolution : 1.95 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

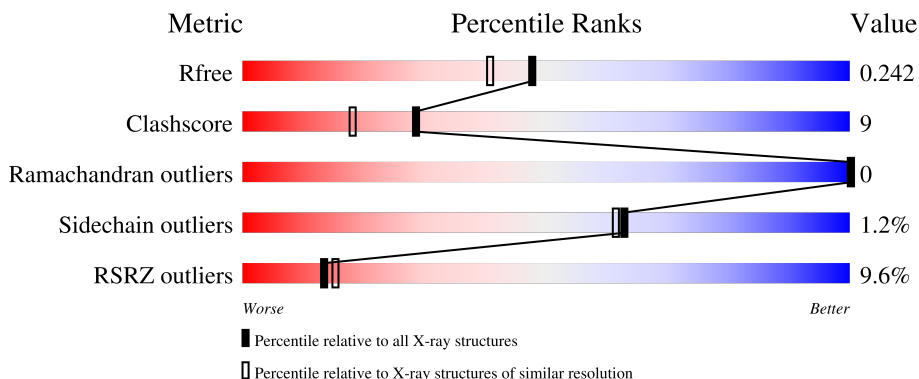
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	621	5% 81% 16% ..
1	B	621	13% 76% 19% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10985 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	608	Total	C	N	O	S	0	0	0
			4872	3090	840	919	23			
1	B	600	Total	C	N	O	S	0	0	0
			4804	3049	832	900	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P00388
B	?	-	GLY	deletion	UNP P00388

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



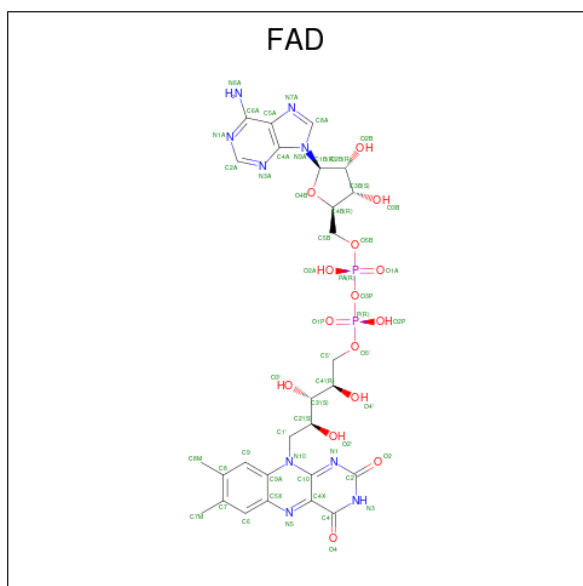
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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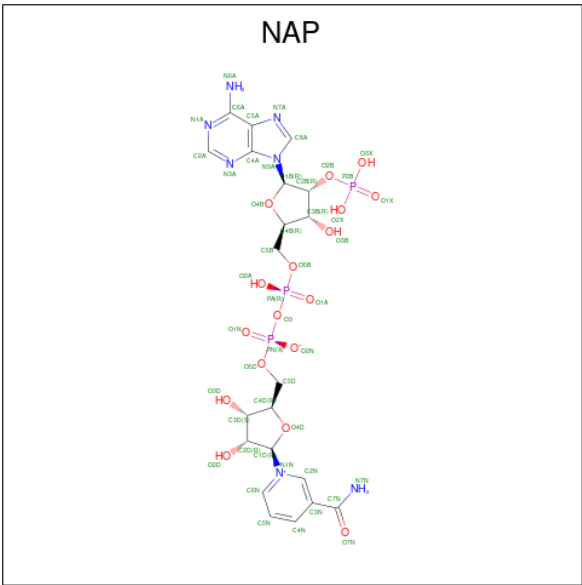
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



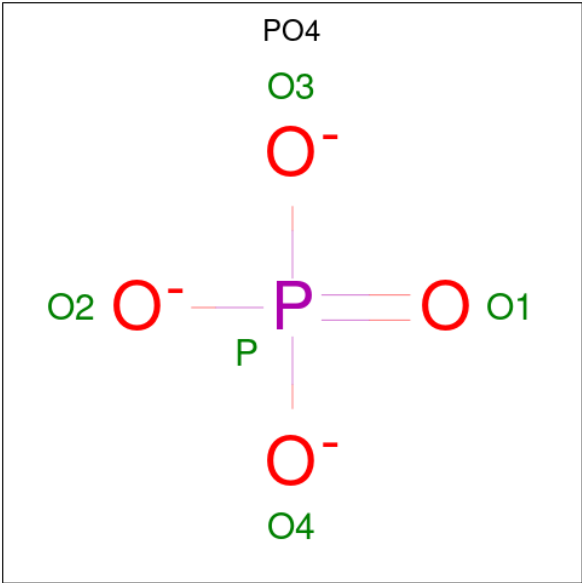
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- 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	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

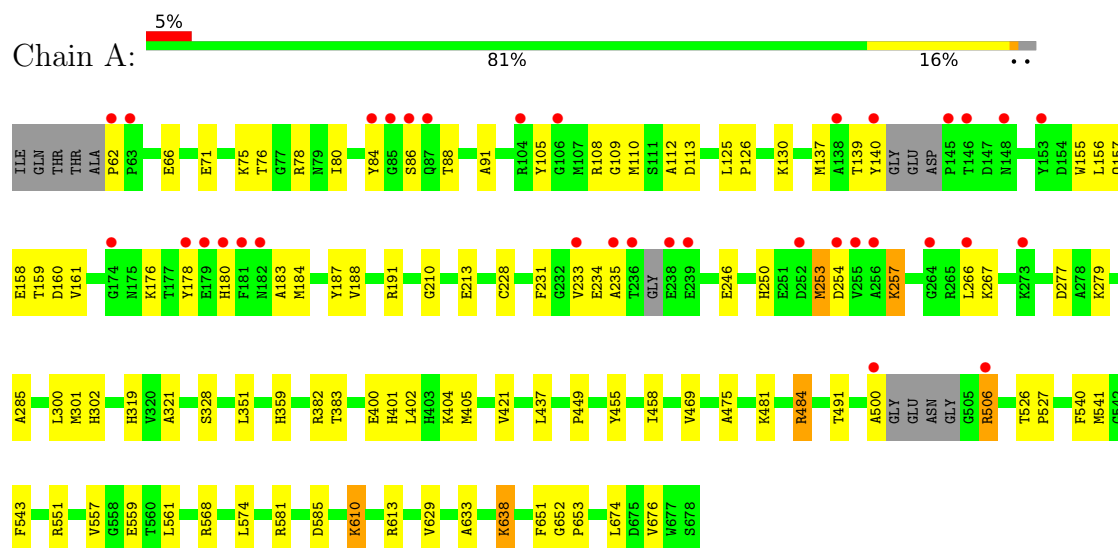
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	609	Total 609	O 609	0	0
6	B	465	Total 465	O 465	0	0

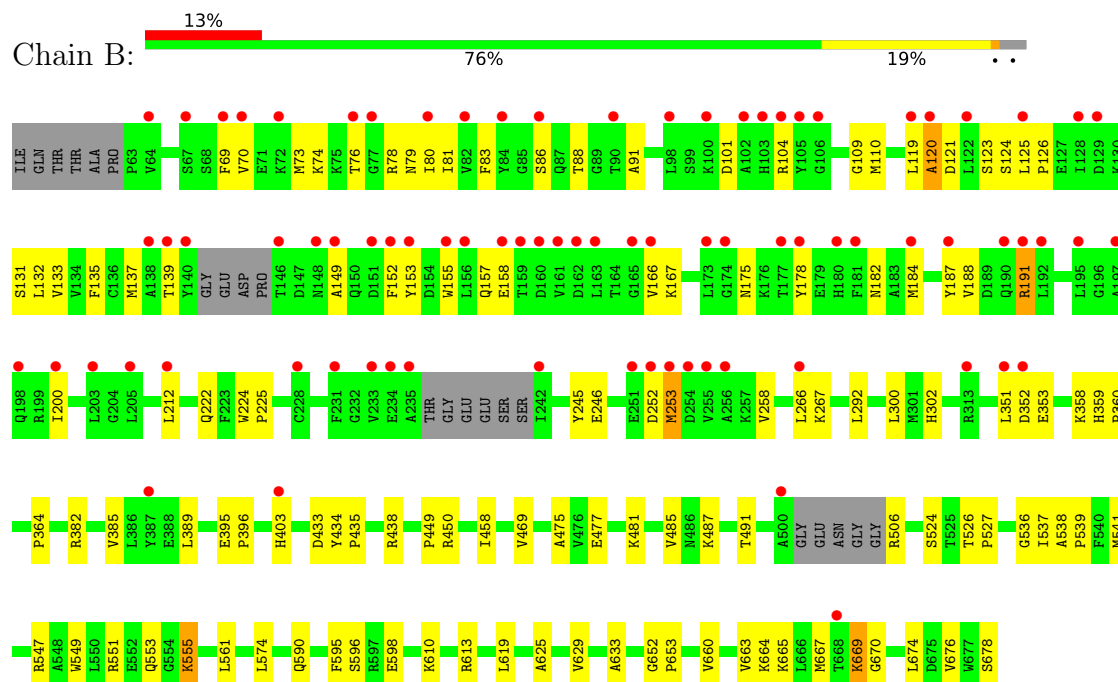
3 Residue-property plots

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	101.79Å 115.05Å 119.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 1.95 47.02 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.02-1.95) 95.5 (47.02-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 1.94Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.203 , 0.241 0.204 , 0.242	Depositor DCC
R_{free} test set	4923 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10985	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.90% 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, FMN, PO4

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	0.45	3/4988 (0.1%)	0.86	9/6747 (0.1%)
1	B	0.40	1/4918 (0.0%)	0.85	12/6651 (0.2%)
All	All	0.43	4/9906 (0.0%)	0.85	21/13398 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	HIS	C-O	-6.66	1.15	1.24
1	A	302	HIS	C-O	-5.73	1.17	1.24
1	B	403	HIS	C-O	-5.27	1.18	1.24
1	A	319	HIS	C-O	-5.16	1.17	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	GLU	N-CA-C	12.18	124.64	111.36
1	B	158	GLU	N-CA-C	7.52	125.15	110.56
1	B	120	ALA	N-CA-C	-7.25	104.44	113.28
1	B	596	SER	N-CA-C	6.61	119.32	111.71
1	B	252	ASP	N-CA-C	5.96	120.61	112.68
1	A	66	GLU	N-CA-C	-5.96	102.84	110.53
1	B	258	VAL	N-CA-C	5.95	116.68	107.99
1	A	421	VAL	N-CA-C	5.74	115.82	110.42
1	A	210	GLY	N-CA-C	-5.71	99.65	113.18
1	B	541	MET	N-CA-C	-5.60	105.26	111.36
1	A	541	MET	N-CA-C	-5.57	105.29	111.36
1	B	158	GLU	CB-CA-C	-5.36	102.41	112.00
1	A	160	ASP	N-CA-C	-5.30	105.09	112.30
1	B	536	GLY	N-CA-C	-5.30	108.84	114.67
1	A	301	MET	N-CA-C	5.28	117.71	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	TYR	CA-C-N	5.21	126.36	119.84
1	B	434	TYR	C-N-CA	5.21	126.36	119.84
1	A	383	THR	N-CA-C	5.12	116.86	111.28
1	B	524	SER	N-CA-C	5.12	117.59	111.71
1	A	137	MET	N-CA-C	5.09	116.81	108.52
1	B	485	VAL	N-CA-C	-5.02	100.03	107.51

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	4872	0	4724	77	0
1	B	4804	0	4650	93	0
2	A	31	0	19	0	0
2	B	31	0	19	2	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	31	0	11	0	0
4	B	31	0	11	0	0
5	B	5	0	0	0	0
6	A	609	0	0	9	0
6	B	465	0	0	9	0
All	All	10985	0	9496	170	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 (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:OG1	1:A:161:VAL:HG13	1.56	1.05
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.53	0.90
1:B:86:SER:HB3	1:B:91:ALA:HB3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:HG1	1:A:161:VAL:HG13	1.44	0.79
1:A:108:ARG:HD2	6:A:1329:HOH:O	1.87	0.74
1:B:125:LEU:HD23	1:B:166:VAL:HG13	1.70	0.72
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.71	0.72
1:A:184:MET:HE2	1:A:188:VAL:HG23	1.71	0.72
1:A:254:ASP:O	1:A:257:LYS:HG2	1.90	0.72
1:B:358:LYS:HD2	1:B:358:LYS:H	1.56	0.70
1:A:228:CYS:HA	1:A:233:VAL:HG12	1.74	0.69
1:B:663:VAL:HG12	1:B:667:MET:HE3	1.75	0.69
1:A:250:HIS:HB3	1:A:253:MET:HG3	1.74	0.68
1:A:254:ASP:HB2	1:A:257:LYS:HD2	1.74	0.68
1:A:184:MET:HE3	1:A:184:MET:HA	1.75	0.68
1:A:638:LYS:HA	1:A:638:LYS:HE3	1.74	0.68
1:B:86:SER:HB2	2:B:701:FMN:O3P	1.96	0.66
1:B:665:LYS:HG2	1:B:669:LYS:HE2	1.78	0.66
1:A:458:ILE:HG23	1:A:469:VAL:HG13	1.80	0.63
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.81	0.63
1:B:629:VAL:HB	1:B:674:LEU:HD23	1.80	0.62
1:B:81:ILE:HD12	1:B:110:MET:HG3	1.81	0.62
1:B:70:VAL:HA	1:B:73:MET:CE	2.29	0.62
1:B:167:LYS:HB3	1:B:200:ILE:CG1	2.30	0.62
1:B:70:VAL:HG21	1:B:124:SER:HB2	1.82	0.61
1:B:70:VAL:HG12	1:B:74:LYS:HE3	1.83	0.61
1:B:104:ARG:HD2	6:B:1007:HOH:O	1.99	0.61
1:A:180:HIS:HB3	1:A:183:ALA:HB2	1.82	0.60
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.31	0.59
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.85	0.59
1:B:88:THR:HB	2:B:701:FMN:O1P	2.03	0.58
1:B:123:SER:O	1:B:126:PRO:HD2	2.03	0.58
1:A:400:GLU:OE2	1:A:404:LYS:HE3	2.04	0.58
1:A:257:LYS:HB2	6:A:899:HOH:O	2.04	0.58
1:B:69:PHE:O	1:B:73:MET:HG3	2.03	0.58
1:B:665:LYS:O	1:B:669:LYS:HD3	2.04	0.58
1:A:321:ALA:HB2	1:A:455:TYR:CE1	2.39	0.57
1:B:69:PHE:CE1	1:B:121:ASP:HB2	2.39	0.57
1:A:285:ALA:HB1	1:A:506:ARG:HE	1.68	0.57
1:A:105:TYR:HD1	1:A:235:ALA:HA	1.69	0.57
1:B:353:GLU:H	1:B:353:GLU:CD	2.13	0.57
1:B:438:ARG:HG3	1:B:438:ARG:HH21	1.69	0.57
1:B:119:LEU:HD22	1:B:152:PHE:CD1	2.40	0.56
1:A:139:THR:O	1:A:140:TYR:CD1	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.87	0.56
1:A:228:CYS:HA	1:A:233:VAL:CG1	2.35	0.56
1:B:477:GLU:HG3	1:B:487:LYS:HD2	1.88	0.55
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.89	0.55
1:B:126:PRO:HA	6:B:818:HOH:O	2.07	0.55
1:B:70:VAL:HA	1:B:73:MET:HE2	1.89	0.55
1:A:561:LEU:HD12	1:A:561:LEU:N	2.22	0.54
1:B:86:SER:HB3	1:B:91:ALA:CB	2.34	0.54
1:A:300:LEU:HD22	1:A:574:LEU:HD21	1.89	0.54
1:A:84:TYR:OH	1:A:113:ASP:HB2	2.07	0.54
1:A:254:ASP:HB2	1:A:257:LYS:CD	2.37	0.53
1:B:449:PRO:HG3	6:B:1233:HOH:O	2.08	0.53
1:B:481:LYS:HE3	6:B:1093:HOH:O	2.08	0.53
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.90	0.53
1:B:222:GLN:C	1:B:225:PRO:HD2	2.32	0.53
1:B:73:MET:HE1	1:B:125:LEU:CD1	2.39	0.53
1:A:449:PRO:HG3	6:A:1382:HOH:O	2.10	0.52
1:B:660:VAL:HG12	1:B:664:LYS:HE3	1.90	0.52
1:B:175:ASN:HB3	1:B:178:TYR:CD2	2.44	0.52
1:B:175:ASN:HB3	1:B:178:TYR:HD2	1.75	0.52
1:A:257:LYS:NZ	1:A:257:LYS:HB3	2.25	0.51
1:B:358:LYS:HD2	1:B:358:LYS:N	2.25	0.51
1:B:78:ARG:HH11	1:B:78:ARG:HG2	1.75	0.51
1:B:101:ASP:HB2	1:B:224:TRP:CZ2	2.45	0.51
1:B:475:ALA:HA	1:B:491:THR:HB	1.92	0.51
1:A:285:ALA:CB	1:A:506:ARG:HE	2.24	0.51
1:B:119:LEU:HD22	1:B:152:PHE:CE1	2.46	0.51
1:B:633:ALA:HB2	1:B:676:VAL:HB	1.94	0.50
1:A:159:THR:OG1	1:A:161:VAL:CG1	2.46	0.50
1:A:250:HIS:CB	1:A:253:MET:HG3	2.41	0.50
1:A:130:LYS:HG3	1:A:231:PHE:CD1	2.47	0.50
1:B:119:LEU:N	1:B:119:LEU:HD12	2.27	0.49
1:B:83:PHE:HB2	1:B:135:PHE:CD1	2.47	0.49
1:B:555:LYS:HB3	1:B:555:LYS:NZ	2.27	0.49
1:A:105:TYR:CD1	1:A:235:ALA:HA	2.47	0.49
1:B:385:VAL:O	1:B:389:LEU:HG	2.12	0.49
1:B:670:GLY:HA2	6:B:903:HOH:O	2.12	0.49
1:B:70:VAL:HA	1:B:73:MET:HE3	1.94	0.49
1:B:137:MET:HG3	1:B:188:VAL:HG21	1.95	0.49
1:A:652:GLY:N	1:A:653:PRO:HA	2.28	0.49
1:B:547:ARG:O	1:B:551:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:LYS:HB3	1:B:200:ILE:HG13	1.96	0.48
1:B:76:THR:HG21	1:B:352:ASP:OD1	2.13	0.48
1:B:266:LEU:HG	1:B:267:LYS:HD3	1.95	0.48
1:B:610:LYS:HE3	6:B:801:HOH:O	2.12	0.48
1:B:80:ILE:O	1:B:109:GLY:HA2	2.14	0.48
1:B:184:MET:O	1:B:188:VAL:HG23	2.14	0.48
1:B:549:TRP:O	1:B:553:GLN:HG2	2.14	0.47
1:A:105:TYR:O	1:A:233:VAL:HG21	2.14	0.47
1:B:246:GLU:HB2	1:B:351:LEU:HD21	1.96	0.47
1:B:132:LEU:HD12	1:B:167:LYS:O	2.15	0.47
1:B:167:LYS:HD2	1:B:200:ILE:HD11	1.97	0.47
1:B:595:PHE:HB3	1:B:598:GLU:HG3	1.96	0.47
1:A:540:PHE:HA	1:A:543:PHE:HB2	1.97	0.47
1:B:506:ARG:HG2	1:B:506:ARG:HH11	1.80	0.47
1:B:678:SER:HA	6:B:889:HOH:O	2.14	0.47
1:A:84:TYR:CE1	1:A:112:ALA:C	2.93	0.47
1:A:78:ARG:CD	1:A:110:MET:HB3	2.45	0.47
1:A:80:ILE:HG23	1:A:109:GLY:HA3	1.97	0.47
1:A:139:THR:C	1:A:140:TYR:CD1	2.92	0.47
1:A:651:PHE:O	1:A:652:GLY:C	2.57	0.46
1:B:79:ASN:O	1:B:131:SER:HA	2.16	0.46
1:B:253:MET:CE	1:B:364:PRO:HG3	2.45	0.46
1:A:157:GLN:HG2	1:A:187:TYR:OH	2.15	0.46
1:A:610:LYS:HE2	1:A:613:ARG:HD3	1.96	0.46
1:B:245:TYR:CE2	1:B:360:PRO:HD3	2.51	0.46
1:A:78:ARG:HD3	1:A:110:MET:HB3	1.97	0.46
1:A:506:ARG:HG2	1:A:506:ARG:HH11	1.80	0.46
1:A:62:PRO:HD3	6:A:1367:HOH:O	2.16	0.46
1:A:233:VAL:HG22	1:A:234:GLU:N	2.30	0.46
1:B:438:ARG:HG3	1:B:438:ARG:NH2	2.31	0.46
1:B:358:LYS:H	1:B:358:LYS:CD	2.28	0.45
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.99	0.45
1:B:191:ARG:O	1:B:191:ARG:HD3	2.16	0.45
1:A:402:LEU:HD11	1:A:437:LEU:HD22	1.97	0.45
1:A:213:GLU:OE1	1:A:382:ARG:HD2	2.16	0.45
1:A:484:ARG:N	1:A:484:ARG:HD2	2.32	0.45
1:A:500:ALA:HB2	1:A:506:ARG:HA	1.97	0.45
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.99	0.45
1:B:664:LYS:HG3	6:B:845:HOH:O	2.16	0.45
1:B:222:GLN:O	1:B:225:PRO:HD2	2.17	0.45
1:A:71:GLU:O	1:A:75:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ASP:C	1:B:435:PRO:HD3	2.41	0.44
1:B:70:VAL:O	1:B:74:LYS:HG3	2.18	0.44
1:B:382:ARG:CZ	6:B:852:HOH:O	2.65	0.44
1:A:559:GLU:HB3	1:A:561:LEU:HD11	1.99	0.44
1:A:125:LEU:N	1:A:126:PRO:CD	2.81	0.44
1:A:257:LYS:NZ	1:A:257:LYS:CB	2.80	0.44
1:B:245:TYR:CD2	1:B:360:PRO:HD3	2.52	0.44
1:B:266:LEU:O	1:B:267:LYS:HB2	2.17	0.44
1:A:76:THR:HB	1:A:78:ARG:NH1	2.32	0.44
1:A:88:THR:HG22	6:A:801:HOH:O	2.17	0.43
1:A:253:MET:CE	1:A:257:LYS:HG3	2.48	0.43
1:A:500:ALA:CB	1:A:506:ARG:HA	2.48	0.43
1:A:475:ALA:HA	1:A:491:THR:HB	2.00	0.43
1:A:257:LYS:HA	1:A:266:LEU:CD2	2.38	0.43
1:B:149:ALA:O	1:B:153:TYR:N	2.41	0.43
1:B:537:ILE:O	1:B:537:ILE:HG13	2.18	0.43
1:B:300:LEU:HD22	1:B:574:LEU:HD21	1.99	0.43
1:B:81:ILE:CD1	1:B:110:MET:HG3	2.48	0.42
1:A:568:ARG:HD2	6:A:1336:HOH:O	2.19	0.42
1:B:652:GLY:N	1:B:653:PRO:HA	2.33	0.42
1:B:458:ILE:HG23	1:B:469:VAL:HG13	2.02	0.42
1:B:526:THR:HA	1:B:527:PRO:HD3	1.86	0.42
1:A:176:LYS:C	1:A:178:TYR:H	2.27	0.42
1:A:526:THR:HA	1:A:527:PRO:HD3	1.89	0.42
1:A:155:TRP:O	1:A:159:THR:HG22	2.20	0.42
1:A:328:SER:HB3	6:A:1284:HOH:O	2.20	0.42
1:B:359:HIS:HB3	1:B:360:PRO:HD2	2.02	0.42
1:B:120:ALA:HA	1:B:155:TRP:CZ2	2.54	0.41
1:A:277:ASP:HB2	6:A:1220:HOH:O	2.19	0.41
1:A:401:HIS:O	1:A:405:MET:HG2	2.20	0.41
1:B:133:VAL:O	1:B:133:VAL:HG13	2.21	0.41
1:B:167:LYS:HB3	1:B:200:ILE:HD11	2.02	0.41
1:A:581:ARG:NH1	1:A:585:ASP:OD2	2.54	0.41
1:A:266:LEU:HG	1:A:267:LYS:HG2	2.03	0.41
1:B:125:LEU:N	1:B:126:PRO:CD	2.84	0.41
1:B:139:THR:OG1	1:B:182:ASN:HA	2.21	0.41
1:B:538:ALA:HB3	1:B:539:PRO:CD	2.50	0.41
1:A:279:LYS:HG2	6:A:1302:HOH:O	2.21	0.41
1:B:360:PRO:O	1:B:450:ARG:HD3	2.21	0.41
1:B:610:LYS:HE2	1:B:613:ARG:HD3	2.03	0.41
1:A:481:LYS:HB3	1:A:481:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:GLN:HG2	1:B:187:TYR:OH	2.21	0.40
1:B:292:LEU:HD11	1:B:302:HIS:HB2	2.03	0.40
1:B:395:GLU:HA	1:B:396:PRO:HD2	1.90	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	600/621 (97%)	586 (98%)	14 (2%)	0	100	100
1	B	592/621 (95%)	570 (96%)	22 (4%)	0	100	100
All	All	1192/1242 (96%)	1156 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	519/531 (98%)	513 (99%)	6 (1%)	63	61
1	B	507/531 (96%)	501 (99%)	6 (1%)	63	61
All	All	1026/1062 (97%)	1014 (99%)	12 (1%)	63	61

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

Mol	Chain	Res	Type
1	A	253	MET
1	A	257	LYS
1	A	484	ARG
1	A	506	ARG
1	A	610	LYS
1	A	638	LYS
1	B	191	ARG
1	B	212	LEU
1	B	253	MET
1	B	555	LYS
1	B	619	LEU
1	B	669	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	244	GLN
1	A	333	GLN
1	A	399	GLN
1	A	465	HIS
1	B	198	GLN
1	B	349	ASN
1	B	359	HIS
1	B	621	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 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
4	NAP	A	703	-	32,33,52	1.63	7 (21%)	50,52,80	1.91	13 (26%)
3	FAD	A	702	-	58,58,58	2.31	13 (22%)	85,89,89	1.95	16 (18%)
4	NAP	B	703	-	32,33,52	1.64	7 (21%)	50,52,80	1.92	13 (26%)
3	FAD	B	702	-	58,58,58	2.30	12 (20%)	85,89,89	1.96	16 (18%)
5	PO4	B	704	-	4,4,4	1.71	0	6,6,6	0.46	0
2	FMN	B	701	-	33,33,33	2.63	13 (39%)	48,50,50	1.62	12 (25%)
2	FMN	A	701	-	33,33,33	2.65	13 (39%)	48,50,50	1.61	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
4	NAP	A	703	-	-	5/21/37/67	0/3/3/5
3	FAD	A	702	-	-	2/34/50/50	0/6/6/6
4	NAP	B	703	-	-	3/21/37/67	0/3/3/5
3	FAD	B	702	-	-	2/34/50/50	0/6/6/6
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3
2	FMN	A	701	-	-	0/18/18/18	0/3/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C8A-N7A	8.56	1.48	1.31
3	B	702	FAD	C8A-N7A	8.51	1.48	1.31
2	B	701	FMN	C8M-C8	-6.88	1.38	1.51
2	A	701	FMN	C8M-C8	-6.54	1.38	1.51
3	A	702	FAD	C8A-N9A	6.21	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C8M-C8	-6.18	1.39	1.51
3	B	702	FAD	C8A-N9A	6.16	1.48	1.37
3	B	702	FAD	C7M-C7	-6.14	1.39	1.51
3	A	702	FAD	C7M-C7	-6.13	1.39	1.51
3	B	702	FAD	C8M-C8	-6.09	1.39	1.51
2	B	701	FMN	C4A-N5	5.25	1.42	1.30
2	A	701	FMN	C4A-N5	5.21	1.42	1.30
2	B	701	FMN	C10-N10	4.95	1.48	1.37
2	B	701	FMN	C9-C9A	4.92	1.47	1.39
2	A	701	FMN	C10-N10	4.89	1.47	1.37
2	A	701	FMN	C9-C9A	4.81	1.47	1.39
2	A	701	FMN	C9A-C5A	4.43	1.48	1.41
2	B	701	FMN	C9A-N10	4.19	1.48	1.41
2	A	701	FMN	C9A-N10	4.18	1.48	1.41
2	B	701	FMN	C9A-C5A	4.11	1.47	1.41
2	A	701	FMN	C8-C7	4.09	1.50	1.40
2	B	701	FMN	C8-C7	3.88	1.50	1.40
3	A	702	FAD	C9A-N10	-3.77	1.34	1.41
3	B	702	FAD	C9A-N10	-3.74	1.34	1.41
4	A	703	NAP	C2A-N1A	3.68	1.40	1.33
3	B	702	FAD	C2A-N3A	3.63	1.40	1.33
4	B	703	NAP	C2A-N3A	3.62	1.40	1.33
3	A	702	FAD	C2A-N3A	3.61	1.40	1.33
4	A	703	NAP	C2A-N3A	3.60	1.40	1.33
4	B	703	NAP	C2A-N1A	3.58	1.40	1.33
3	A	702	FAD	C2A-N1A	3.56	1.40	1.33
3	A	702	FAD	C10-N1	3.55	1.40	1.33
3	B	702	FAD	C2A-N1A	3.54	1.40	1.33
3	B	702	FAD	C10-N1	3.52	1.40	1.33
2	B	701	FMN	C10-N1	3.18	1.39	1.33
2	A	701	FMN	C10-N1	3.13	1.39	1.33
4	B	703	NAP	C5A-C4A	-3.09	1.33	1.39
4	A	703	NAP	C5A-N7A	-3.08	1.33	1.39
4	A	703	NAP	C5A-C4A	-3.04	1.33	1.39
3	A	702	FAD	C5A-N7A	-3.02	1.33	1.39
4	B	703	NAP	C5A-N7A	-3.01	1.33	1.39
2	A	701	FMN	C4'-C3'	2.98	1.58	1.53
3	B	702	FAD	C5A-N7A	-2.97	1.33	1.39
3	A	702	FAD	C5A-C4A	-2.92	1.33	1.39
2	B	701	FMN	C6-C5A	2.89	1.44	1.40
3	B	702	FAD	C5A-C4A	-2.88	1.33	1.39
2	A	701	FMN	C1'-C2'	2.88	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C5X-N5	-2.69	1.34	1.39
3	B	702	FAD	C5A-C6A	-2.68	1.33	1.41
3	B	702	FAD	C5X-N5	-2.68	1.34	1.39
3	A	702	FAD	C5A-C6A	-2.66	1.33	1.41
4	A	703	NAP	C5A-C6A	-2.64	1.33	1.41
2	A	701	FMN	C6-C5A	2.63	1.44	1.40
2	A	701	FMN	O2'-C2'	2.63	1.48	1.43
4	B	703	NAP	C5A-C6A	-2.62	1.33	1.41
2	B	701	FMN	O2'-C2'	2.58	1.48	1.43
2	B	701	FMN	C4'-C3'	2.52	1.57	1.53
4	A	703	NAP	C8A-N9A	-2.40	1.33	1.37
4	B	703	NAP	C8A-N9A	-2.39	1.33	1.37
2	B	701	FMN	C7M-C7	2.17	1.55	1.51
2	B	701	FMN	C1'-C2'	2.14	1.55	1.52
2	A	701	FMN	C7M-C7	2.05	1.54	1.51
3	A	702	FAD	C4A-N9A	-2.04	1.33	1.37
4	A	703	NAP	C4A-N9A	-2.04	1.33	1.37
4	B	703	NAP	C4A-N9A	-2.03	1.33	1.37

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N9A-C8A-N7A	-9.47	100.50	113.94
3	B	702	FAD	N9A-C8A-N7A	-9.39	100.61	113.94
3	A	702	FAD	N3A-C2A-N1A	-7.43	117.34	128.58
3	B	702	FAD	N3A-C2A-N1A	-7.29	117.55	128.58
4	A	703	NAP	N3A-C2A-N1A	-7.19	117.69	128.58
4	B	703	NAP	N3A-C2A-N1A	-7.19	117.70	128.58
3	B	702	FAD	C5A-C4A-N3A	-4.60	120.38	126.72
4	B	703	NAP	N9A-C8A-N7A	-4.38	107.73	113.94
4	A	703	NAP	N9A-C8A-N7A	-4.26	107.89	113.94
3	A	702	FAD	C5A-C4A-N3A	-4.26	120.85	126.72
4	B	703	NAP	C5A-C4A-N3A	-4.22	120.91	126.72
3	B	702	FAD	C5A-C4A-N9A	4.18	110.36	105.81
4	A	703	NAP	C5A-C4A-N3A	-4.15	121.00	126.72
3	A	702	FAD	C5A-C4A-N9A	3.96	110.12	105.81
2	B	701	FMN	C9A-C5A-N5	3.94	126.64	122.45
2	A	701	FMN	C9A-C5A-N5	3.93	126.63	122.45
2	A	701	FMN	O4'-C4'-C3'	-3.56	100.91	109.25
3	B	702	FAD	C2A-N3A-C4A	3.55	120.51	111.83
2	B	701	FMN	O4'-C4'-C3'	-3.52	101.01	109.25
3	A	702	FAD	C2A-N3A-C4A	3.49	120.35	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	C5A-N7A-C8A	3.43	108.84	103.45
3	B	702	FAD	C5A-N7A-C8A	3.43	108.84	103.45
4	B	703	NAP	C2A-N3A-C4A	3.31	119.91	111.83
4	A	703	NAP	C2A-N3A-C4A	3.27	119.83	111.83
4	B	703	NAP	C5A-N7A-C8A	3.18	108.45	103.45
3	A	702	FAD	C4-N3-C2	-3.08	120.18	125.64
4	A	703	NAP	C5A-N7A-C8A	3.05	108.24	103.45
3	B	702	FAD	C4-N3-C2	-3.00	120.31	125.64
3	A	702	FAD	C4A-N9A-C8A	2.98	108.87	105.74
2	B	701	FMN	O3P-P-O5'	-2.88	99.15	106.67
3	A	702	FAD	C5A-C6A-N6A	-2.84	116.25	123.29
3	B	702	FAD	C5A-C6A-N6A	-2.82	116.30	123.29
2	B	701	FMN	C5A-C9A-N10	-2.82	115.42	117.97
3	B	702	FAD	C4A-N9A-C8A	2.78	108.66	105.74
2	A	701	FMN	C5A-C9A-N10	-2.77	115.47	117.97
2	A	701	FMN	C4'-C3'-C2'	-2.76	108.98	113.57
3	B	702	FAD	C10-C4X-N5	-2.73	119.23	124.81
2	B	701	FMN	O4-C4-N3	-2.71	115.02	120.11
4	B	703	NAP	C4A-C5A-N7A	-2.70	107.50	110.58
3	A	702	FAD	C10-C4X-N5	-2.64	119.41	124.81
2	A	701	FMN	C8M-C8-C7	2.63	126.14	120.76
3	A	702	FAD	C4X-C4-N3	2.58	119.82	113.25
3	B	702	FAD	C4X-C4-N3	2.56	119.78	113.25
4	A	703	NAP	C5A-C6A-N6A	-2.56	116.94	123.29
2	B	701	FMN	C8M-C8-C7	2.56	125.98	120.76
2	A	701	FMN	O4-C4-N3	-2.56	115.31	120.11
2	A	701	FMN	C5A-N5-C4A	-2.53	113.99	118.09
4	B	703	NAP	C6A-C5A-C4A	2.50	120.59	117.18
4	A	703	NAP	C6A-C5A-C4A	2.50	120.59	117.18
3	B	702	FAD	C2B-C3B-C4B	-2.49	97.79	102.61
3	A	702	FAD	C2B-C3B-C4B	-2.48	97.82	102.61
4	B	703	NAP	C5A-C6A-N6A	-2.47	117.18	123.29
4	A	703	NAP	C4A-C5A-N7A	-2.47	107.76	110.58
2	B	701	FMN	C5A-N5-C4A	-2.43	114.15	118.09
3	A	702	FAD	C4X-C10-N10	2.43	119.96	116.48
3	B	702	FAD	C6A-C5A-C4A	2.38	120.43	117.18
4	B	703	NAP	C3B-C2B-C1B	-2.38	98.25	102.81
2	A	701	FMN	O3P-P-O5'	-2.37	100.49	106.67
3	B	702	FAD	C4X-C10-N10	2.35	119.84	116.48
2	A	701	FMN	C8M-C8-C9	-2.34	115.44	119.57
2	B	701	FMN	C4'-C3'-C2'	-2.34	109.68	113.57
2	B	701	FMN	O2P-P-O1P	2.33	119.91	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	FAD	C9A-C5X-N5	-2.30	120.01	122.45
2	B	701	FMN	C8M-C8-C9	-2.26	115.59	119.57
2	A	701	FMN	C7M-C7-C6	-2.25	115.61	119.57
3	A	702	FAD	O4-C4-C4X	-2.25	120.60	126.53
4	B	703	NAP	C5A-C4A-N9A	2.24	108.26	105.81
3	B	702	FAD	O4-C4-C4X	-2.24	120.63	126.53
2	A	701	FMN	O2P-P-O1P	2.23	119.54	110.83
2	B	701	FMN	C9-C9A-N10	2.22	124.84	121.85
4	A	703	NAP	N3A-C4A-N9A	2.21	130.93	127.17
3	A	702	FAD	C9A-C5X-N5	-2.19	120.13	122.45
2	B	701	FMN	C7M-C7-C6	-2.19	115.71	119.57
4	A	703	NAP	C3B-C2B-C1B	-2.19	98.61	102.81
4	A	703	NAP	C4A-N9A-C8A	2.19	108.03	105.74
4	B	703	NAP	C4A-N9A-C8A	2.19	108.03	105.74
4	B	703	NAP	N3A-C4A-N9A	2.15	130.83	127.17
2	A	701	FMN	C9-C9A-N10	2.13	124.72	121.85
4	A	703	NAP	O2N-PN-O1N	2.12	119.09	110.83
3	A	702	FAD	C6A-C5A-C4A	2.10	120.05	117.18
4	B	703	NAP	O2N-PN-O1N	2.08	118.93	110.83
4	A	703	NAP	C5A-C4A-N9A	2.06	108.06	105.81

There are no chirality outliers.

All (12) torsion outliers are listed below:

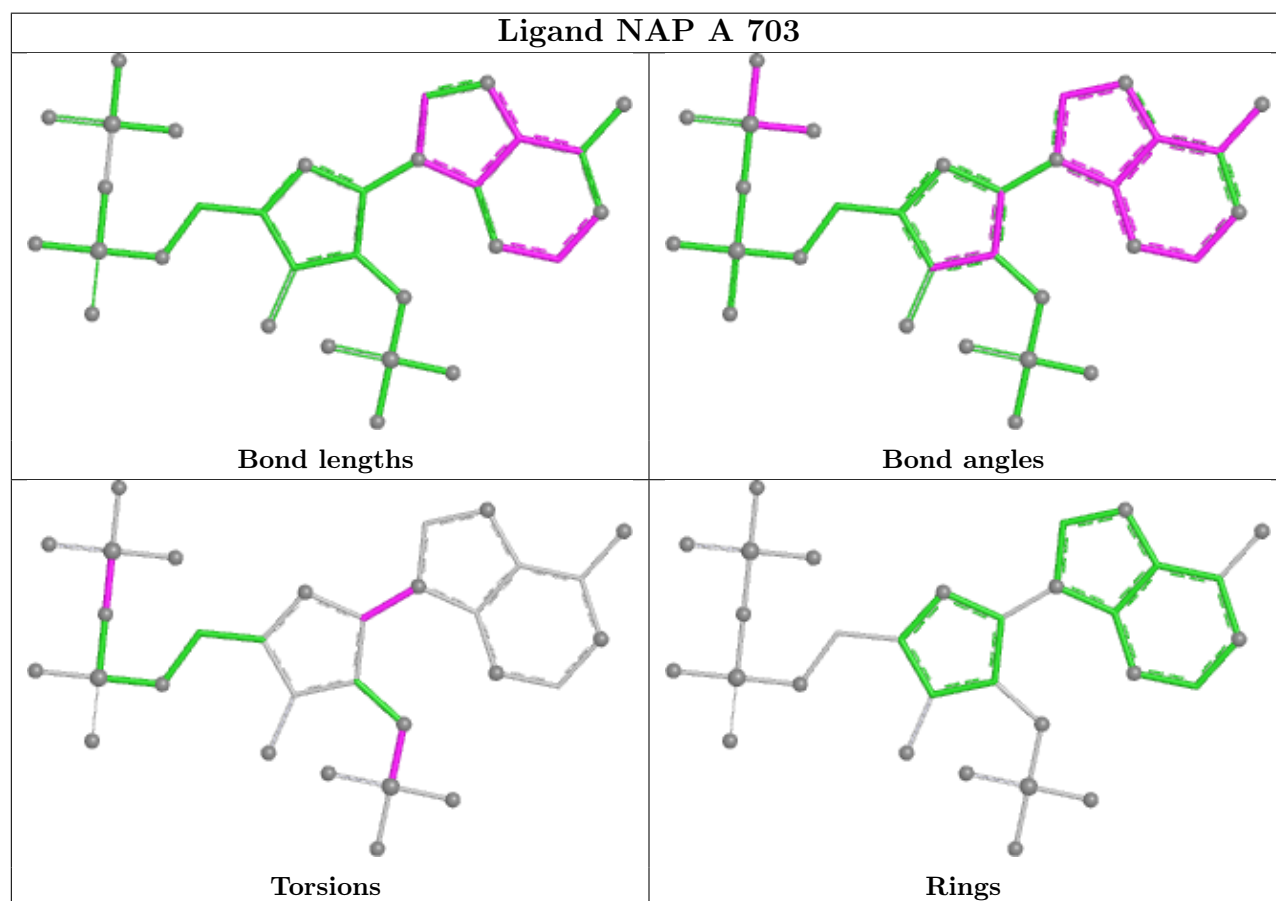
Mol	Chain	Res	Type	Atoms
4	A	703	NAP	C2B-C1B-N9A-C8A
4	A	703	NAP	PA-O3-PN-O2N
4	B	703	NAP	C2B-C1B-N9A-C8A
4	A	703	NAP	C2B-C1B-N9A-C4A
4	B	703	NAP	C2B-C1B-N9A-C4A
4	A	703	NAP	PA-O3-PN-O1N
4	A	703	NAP	C2B-O2B-P2B-O1X
4	B	703	NAP	C2B-O2B-P2B-O1X
3	A	702	FAD	PA-O3P-P-O1P
3	B	702	FAD	PA-O3P-P-O1P
3	A	702	FAD	PA-O3P-P-O2P
3	B	702	FAD	PA-O3P-P-O2P

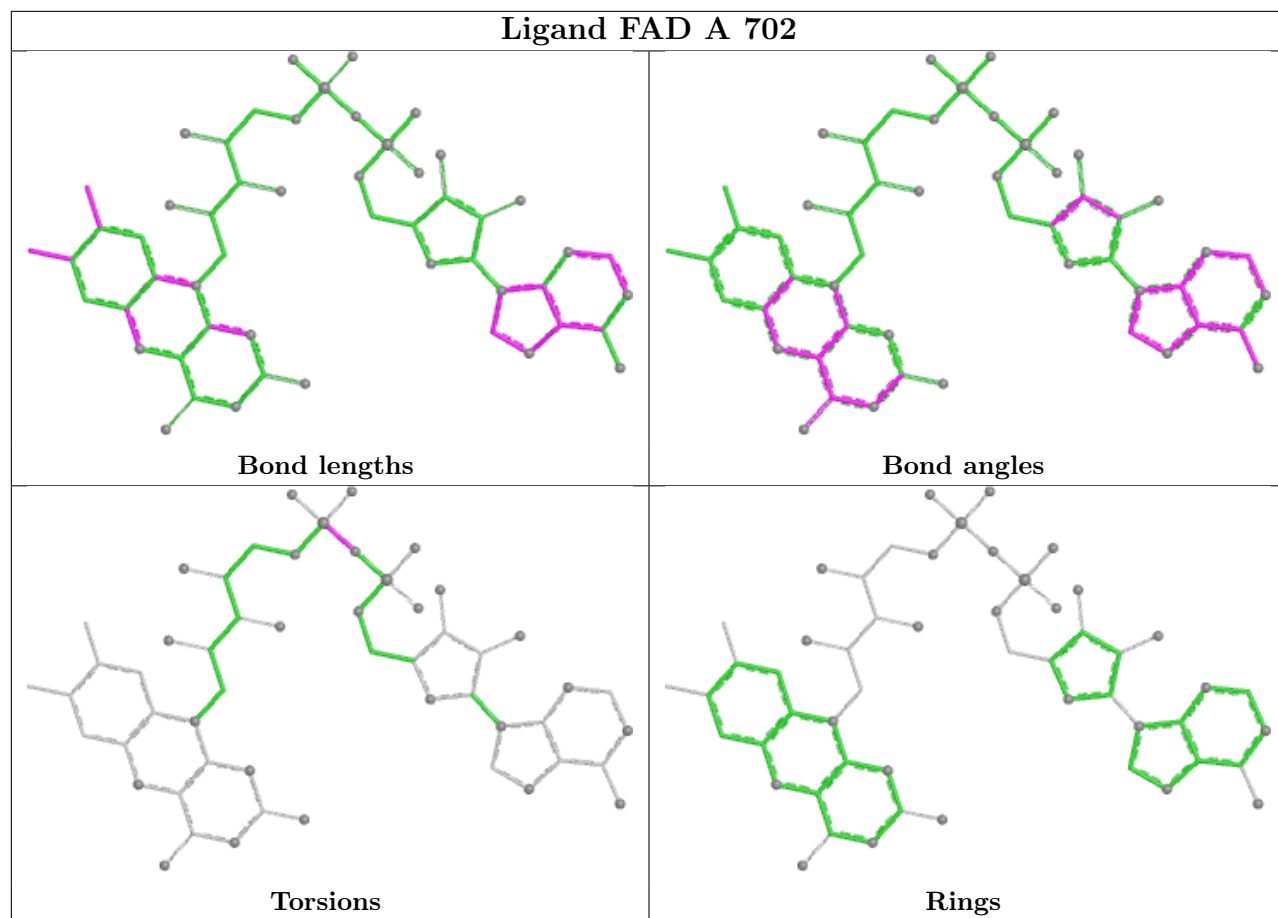
There are no ring outliers.

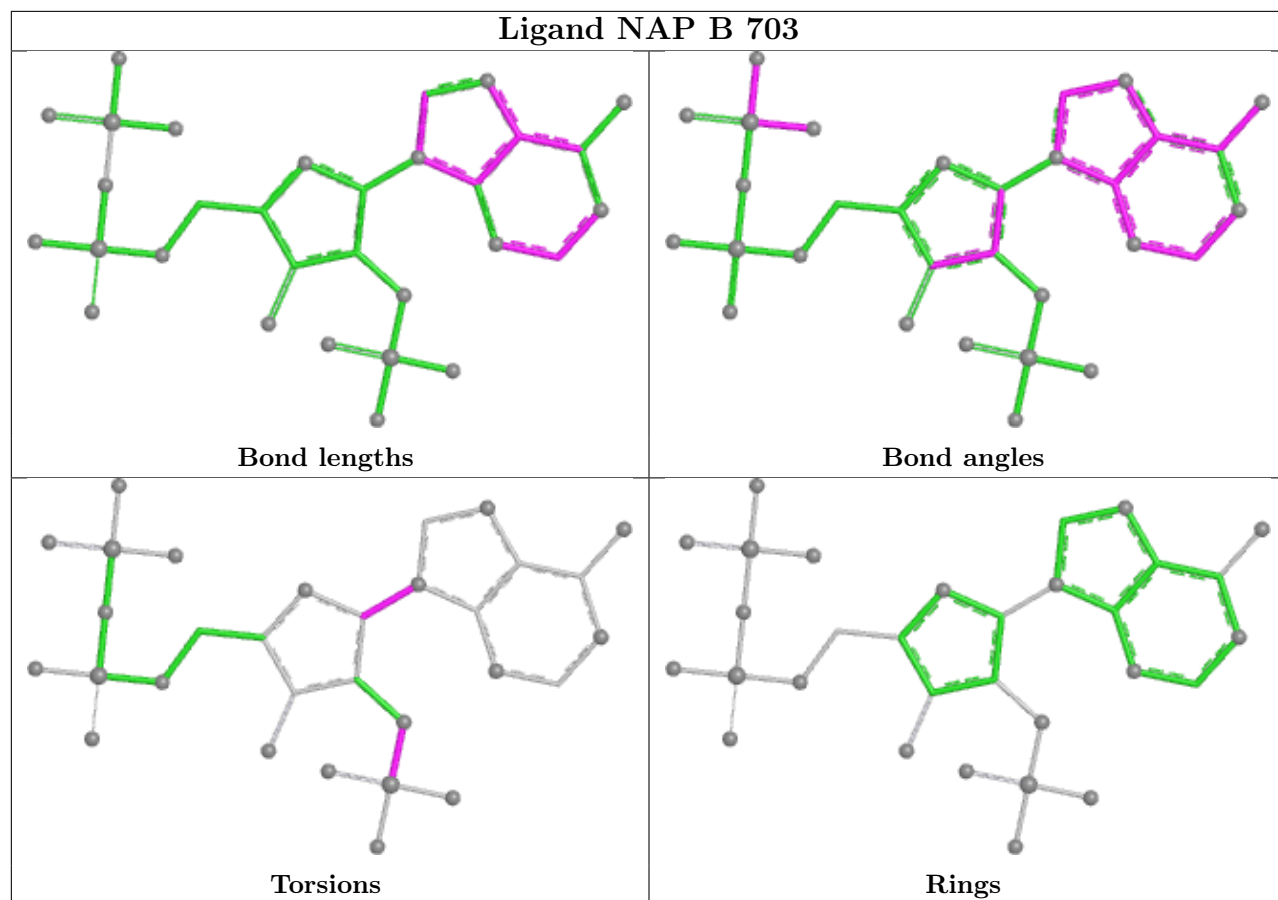
1 monomer is involved in 2 short contacts:

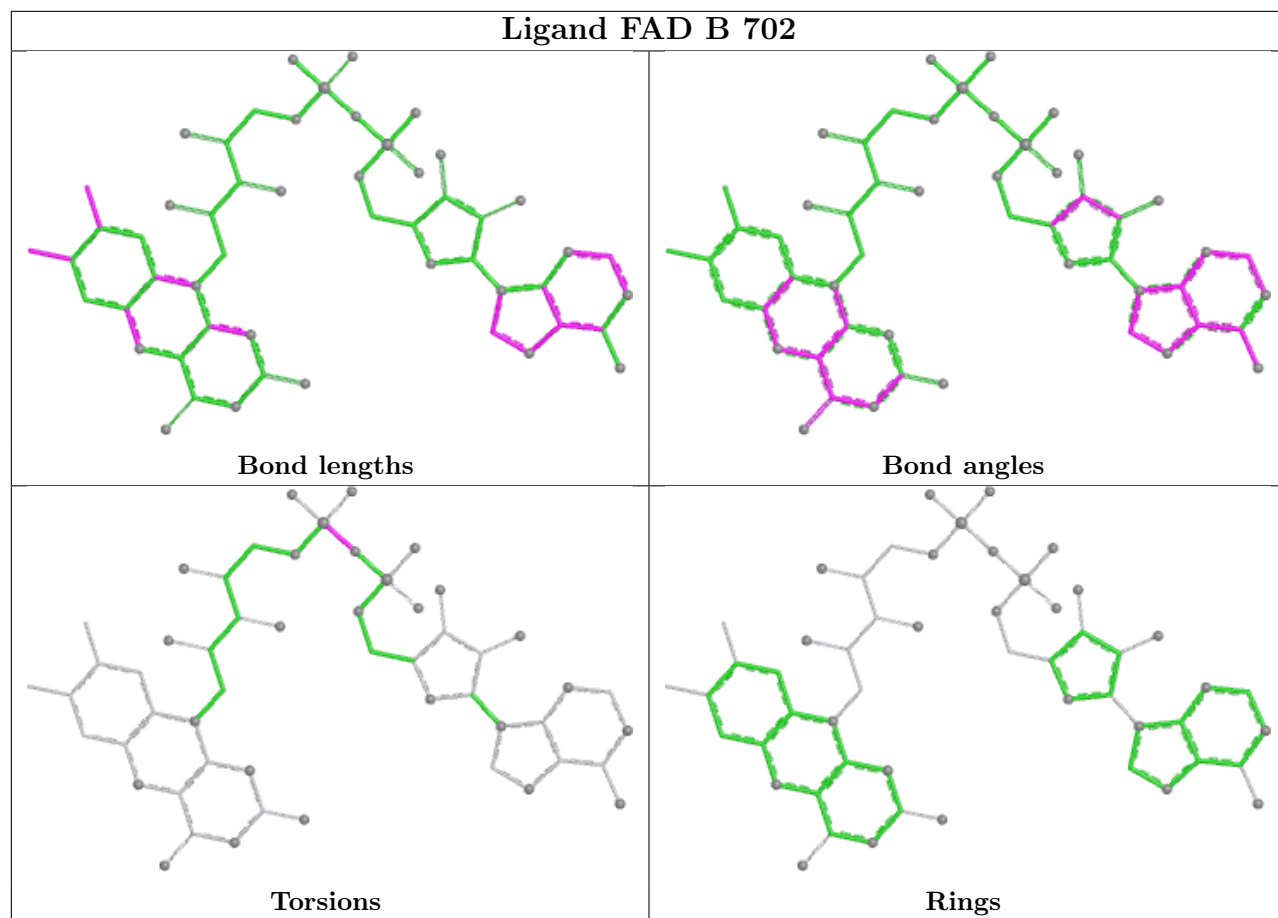
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FMN	2	0

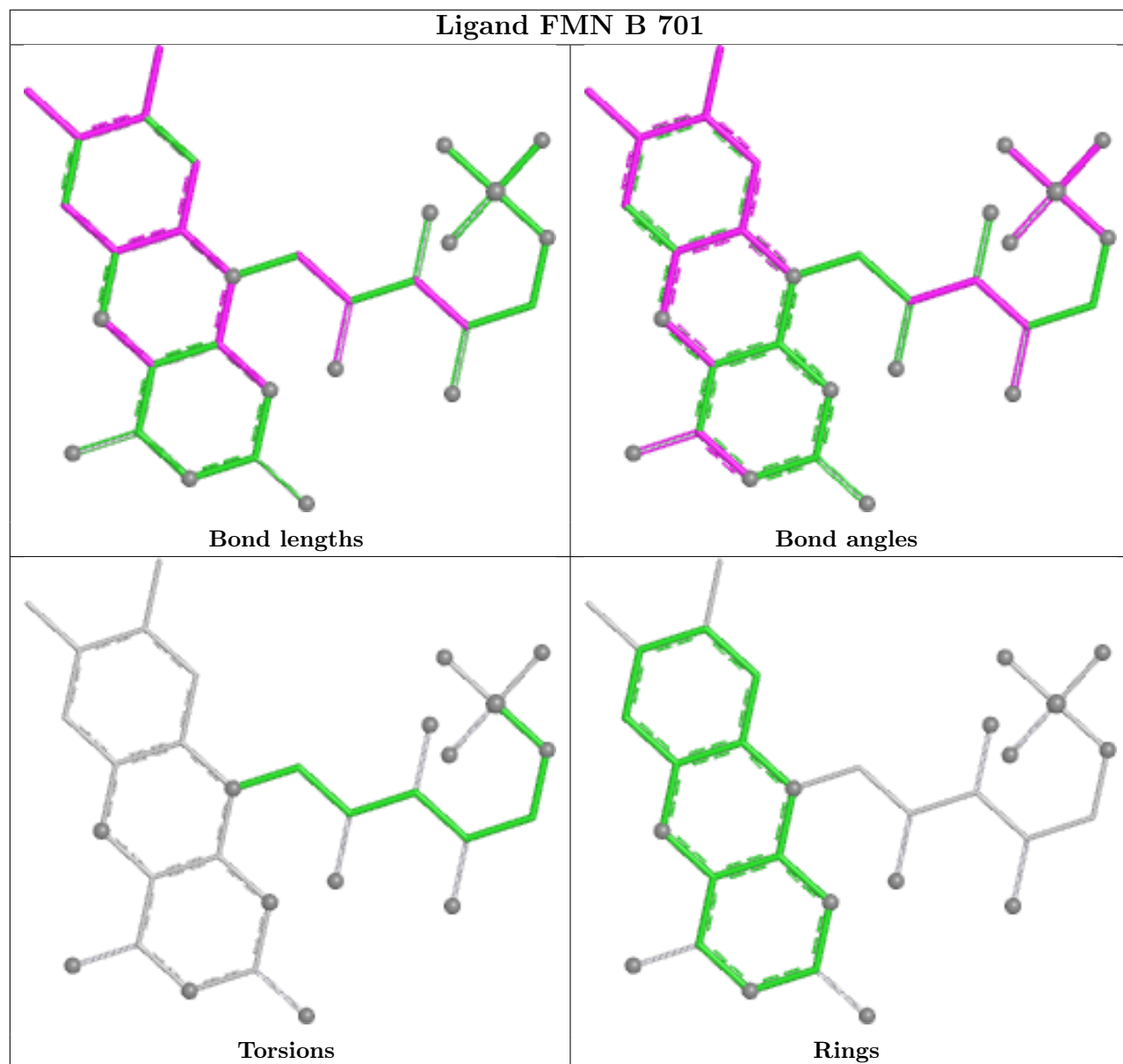
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

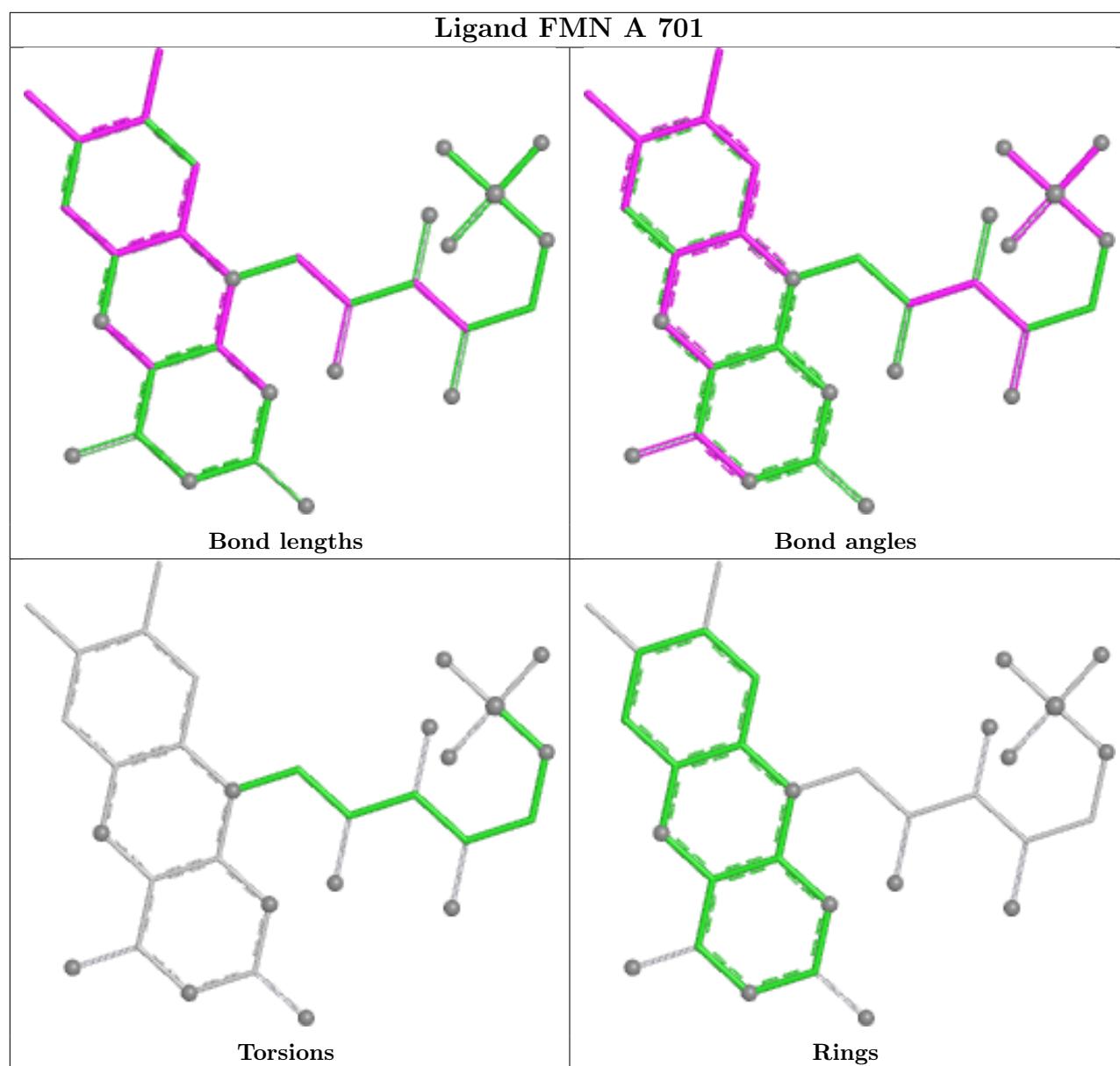












5.7 Other polymers [i](#)

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	608/621 (97%)	0.29	34 (5%) 30 35	22, 32, 52, 81	0
1	B	600/621 (96%)	0.70	82 (13%) 6 7	22, 36, 71, 101	0
All	All	1208/1242 (97%)	0.50	116 (9%) 13 15	22, 33, 67, 101	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	VAL	5.5
1	B	233	VAL	4.7
1	A	145	PRO	4.6
1	B	200	ILE	4.4
1	B	152	PHE	4.3
1	A	140	TYR	4.2
1	B	155	TRP	4.2
1	B	146	THR	4.2
1	B	149	ALA	4.1
1	B	159	THR	4.0
1	A	180	HIS	3.9
1	B	128	ILE	3.9
1	B	192	LEU	3.8
1	A	235	ALA	3.8
1	B	120	ALA	3.7
1	A	236	THR	3.7
1	B	255	VAL	3.7
1	A	85	GLY	3.7
1	B	235	ALA	3.6
1	B	181	PHE	3.6
1	B	148	ASN	3.5
1	A	500	ALA	3.5
1	B	252	ASP	3.5
1	B	119	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	3.4
1	B	156	LEU	3.3
1	A	62	PRO	3.3
1	B	138	ALA	3.3
1	A	252	ASP	3.3
1	A	178	TYR	3.2
1	A	63	PRO	3.2
1	B	140	TYR	3.2
1	B	351	LEU	3.2
1	B	104	ARG	3.2
1	B	253	MET	3.1
1	B	403	HIS	3.1
1	A	84	TYR	3.1
1	B	163	LEU	3.0
1	B	162	ASP	3.0
1	B	197	ALA	3.0
1	B	234	GLU	3.0
1	B	191	ARG	3.0
1	A	256	ALA	2.9
1	B	190	GLN	2.9
1	B	165	GLY	2.9
1	B	173	LEU	2.9
1	B	242	ILE	2.9
1	A	174	GLY	2.9
1	B	125	LEU	2.8
1	B	129	ASP	2.8
1	B	180	HIS	2.8
1	A	146	THR	2.8
1	A	179	GLU	2.8
1	B	251	GLU	2.7
1	B	122	LEU	2.7
1	A	238	GLU	2.7
1	A	273	LYS	2.7
1	A	138	ALA	2.6
1	B	500	ALA	2.6
1	A	148	ASN	2.6
1	B	106	GLY	2.6
1	B	82	VAL	2.6
1	A	153	TYR	2.6
1	B	153	TYR	2.6
1	B	178	TYR	2.6
1	B	352	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	239	GLU	2.5
1	B	254	ASP	2.5
1	B	151	ASP	2.5
1	A	266	LEU	2.5
1	B	166	VAL	2.5
1	A	181	PHE	2.5
1	A	506	ARG	2.5
1	A	182	ASN	2.4
1	B	105	TYR	2.4
1	B	139	THR	2.4
1	B	103	HIS	2.4
1	B	184	MET	2.4
1	B	70	VAL	2.4
1	B	174	GLY	2.4
1	B	160	ASP	2.4
1	A	264	GLY	2.4
1	B	98	LEU	2.3
1	A	254	ASP	2.3
1	B	100	LYS	2.2
1	A	104	ARG	2.2
1	B	313	ARG	2.2
1	B	198	GLN	2.2
1	B	187	TYR	2.2
1	B	231	PHE	2.2
1	B	228	CYS	2.2
1	B	203	LEU	2.2
1	B	205	LEU	2.2
1	B	212	LEU	2.2
1	B	266	LEU	2.2
1	B	102	ALA	2.2
1	B	76	THR	2.1
1	B	90	THR	2.1
1	B	67	SER	2.1
1	A	106	GLY	2.1
1	B	158	GLU	2.1
1	B	86	SER	2.1
1	B	177	THR	2.1
1	B	387	TYR	2.1
1	B	77	GLY	2.1
1	A	255	VAL	2.1
1	A	87	GLN	2.1
1	B	69	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	80	ILE	2.0
1	B	84	TYR	2.0
1	B	668	THR	2.0
1	B	256	ALA	2.0
1	B	72	LYS	2.0
1	A	86	SER	2.0
1	A	233	VAL	2.0
1	B	64	VAL	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

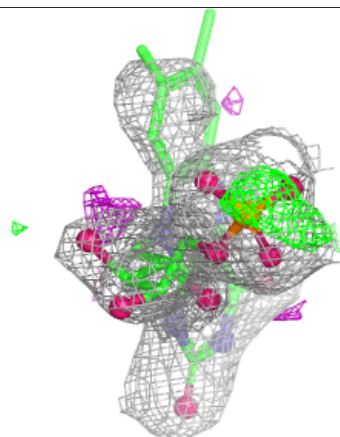
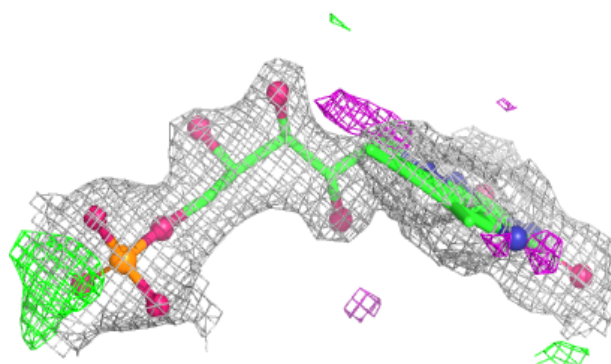
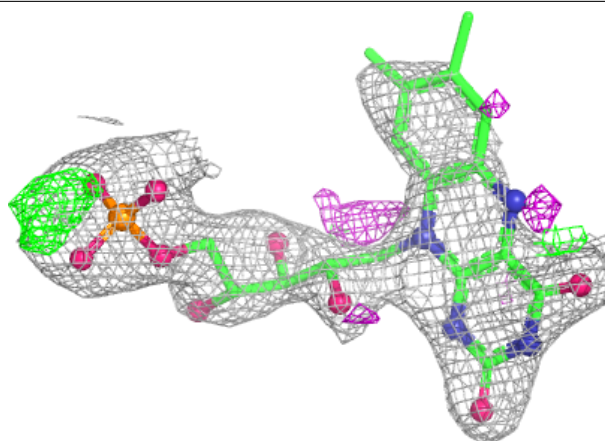
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	B	704	5/5	0.63	0.17	106,106,107,107	0
2	FMN	B	701	31/31	0.83	0.15	60,70,74,74	0
2	FMN	A	701	31/31	0.92	0.09	32,38,41,43	0
4	NAP	B	703	31/48	0.96	0.06	21,25,42,50	0
3	FAD	B	702	53/53	0.97	0.06	20,24,32,33	0
4	NAP	A	703	31/48	0.97	0.05	22,24,36,46	0
3	FAD	A	702	53/53	0.98	0.05	21,25,32,37	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.

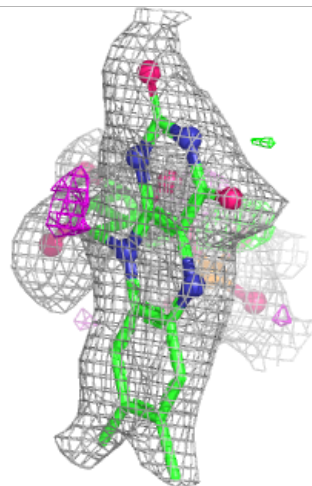
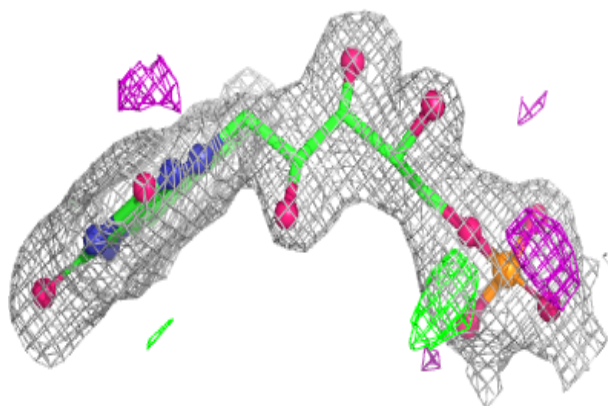
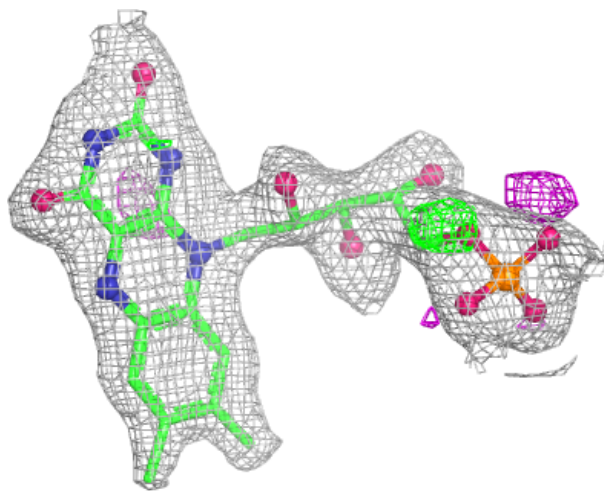
Electron density around FMN B 701:

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



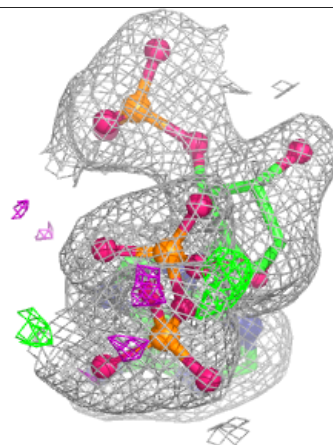
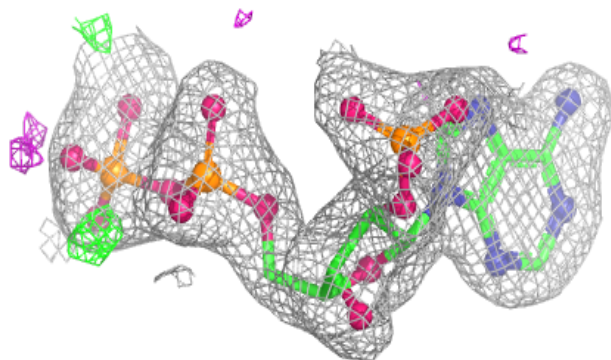
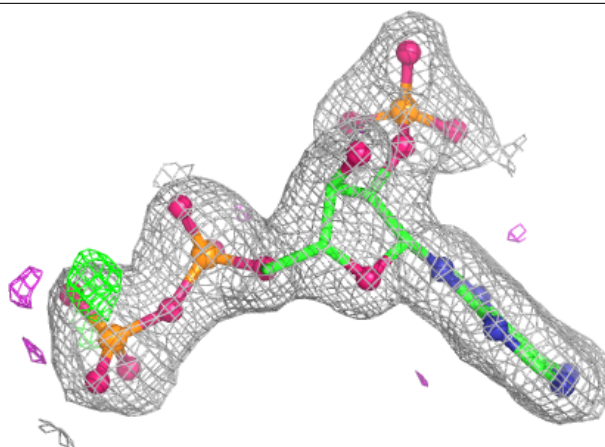
Electron density around FMN A 701:

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

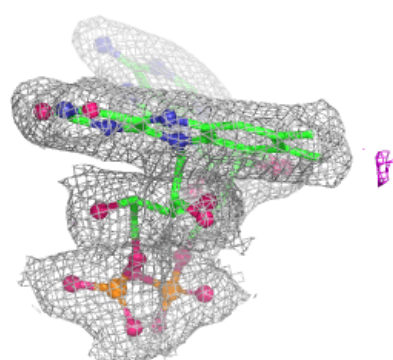
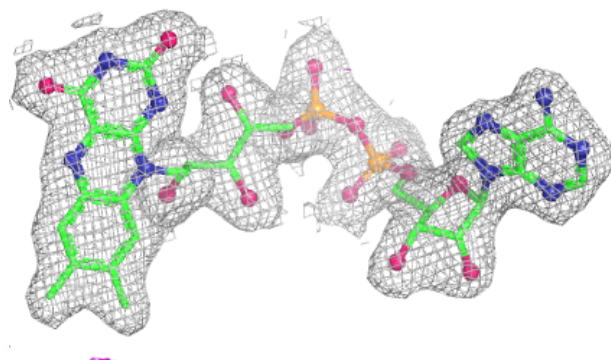
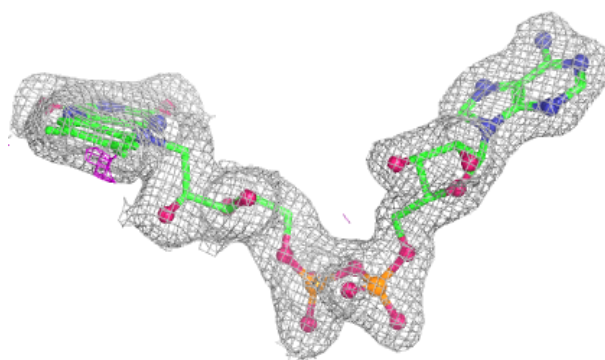


Electron density around NAP B 703:

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

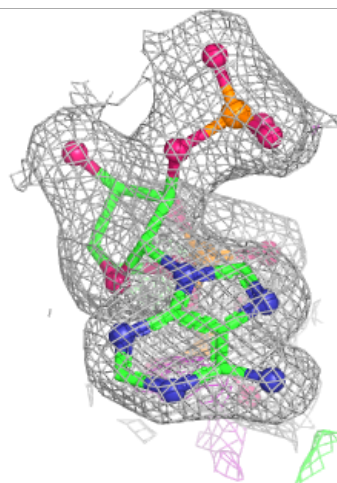
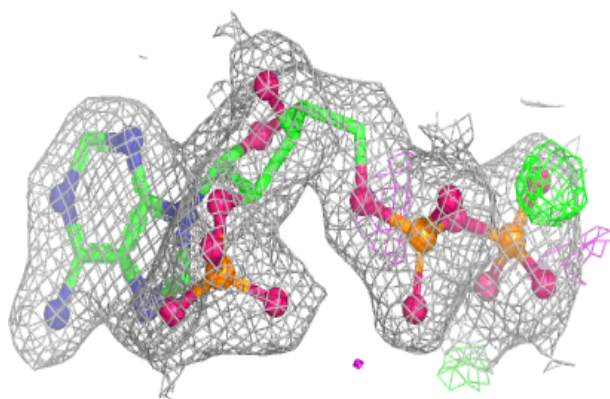
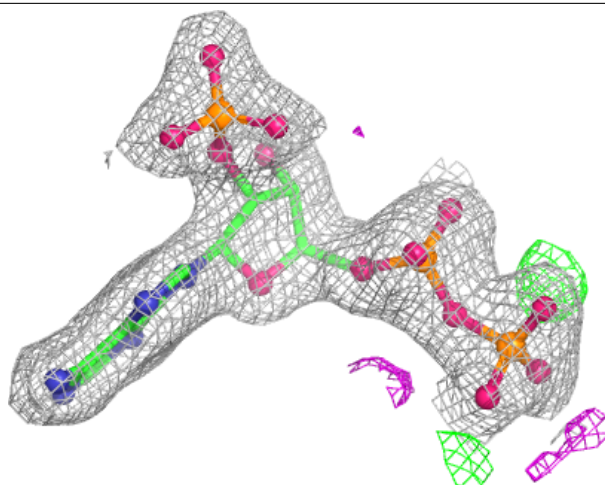
**Electron density around FAD B 702:**

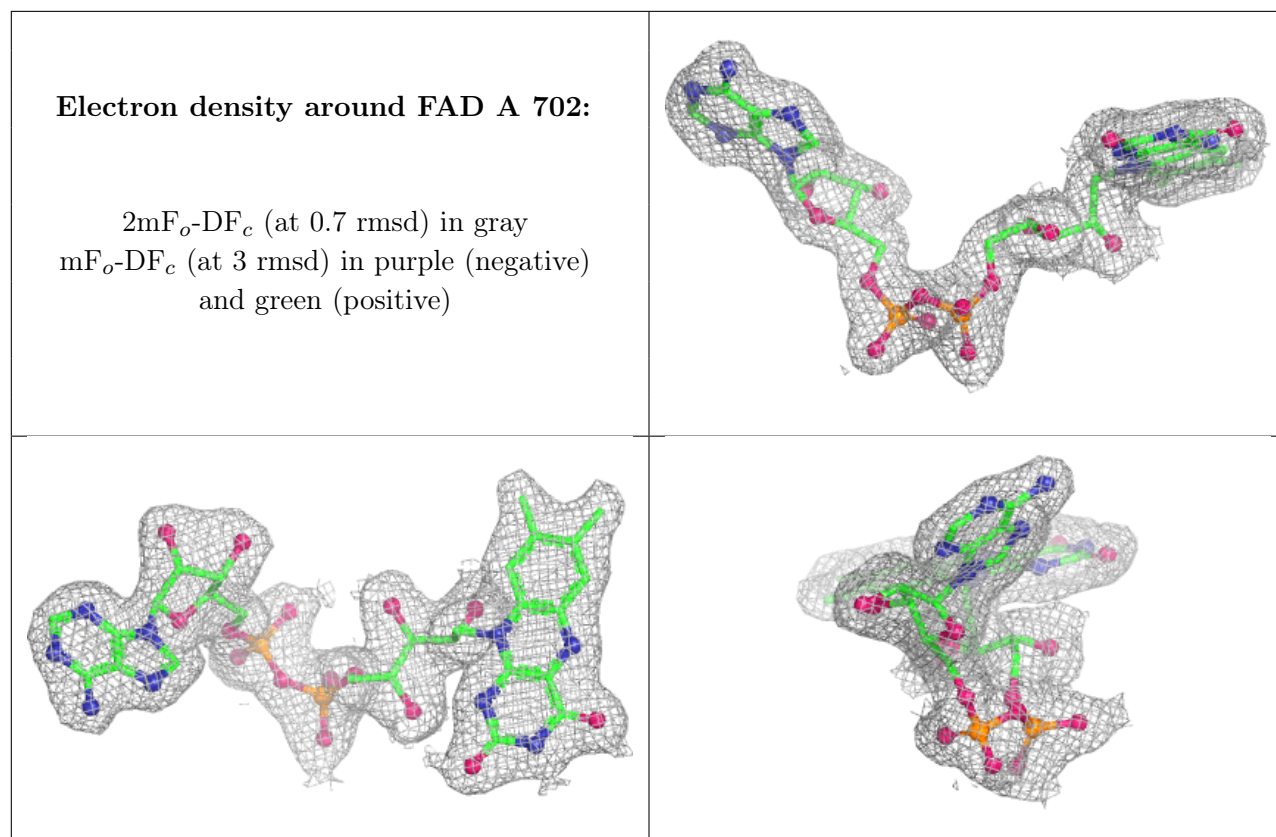
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.