



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:14 PM UTC

PDB ID : 1J9Z / pdb_00001j9z
Title : CYPOR-W677G
Authors : Hubbard, P.A.; Shen, A.L.; Paschke, R.; Kasper, C.B.; Kim, J.J.
Deposited on : 2001-05-29
Resolution : 2.70 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

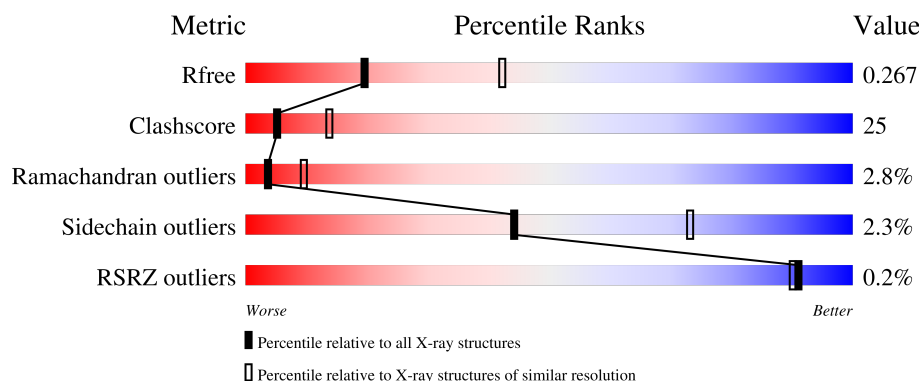
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 5 unique types of molecules in this entry. The entry contains 10265 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.

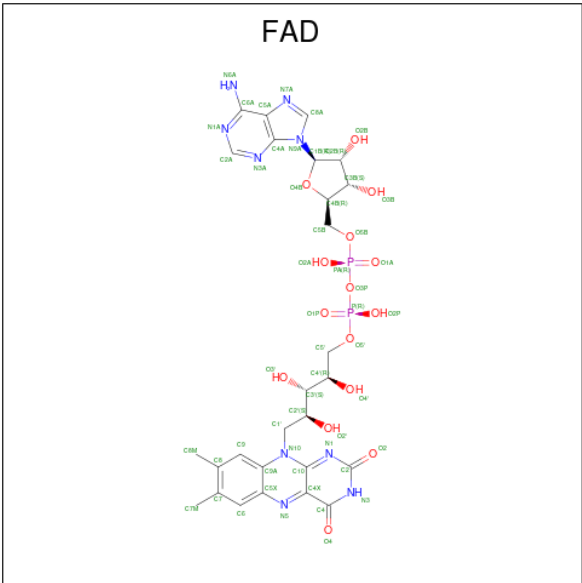
- Molecule 1 is a protein called NADPH-Cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4901	3099	844	935	23			
1	B	611	Total	C	N	O	S	0	0	0
			4890	3092	842	933	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	GLY	TRP	engineered mutation	UNP P00388
B	677	GLY	TRP	engineered mutation	UNP P00388

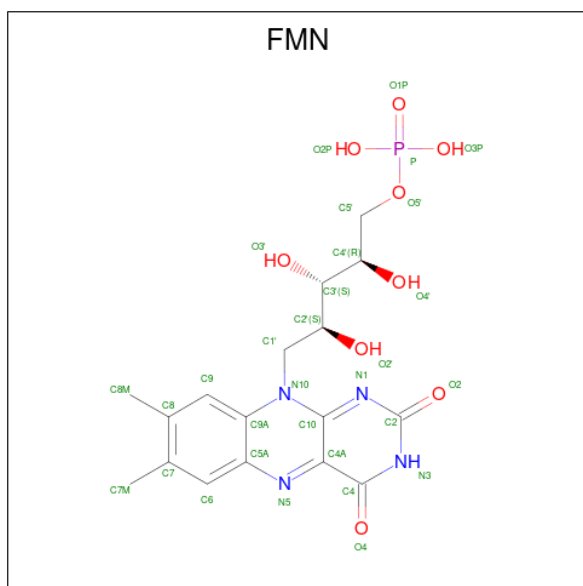
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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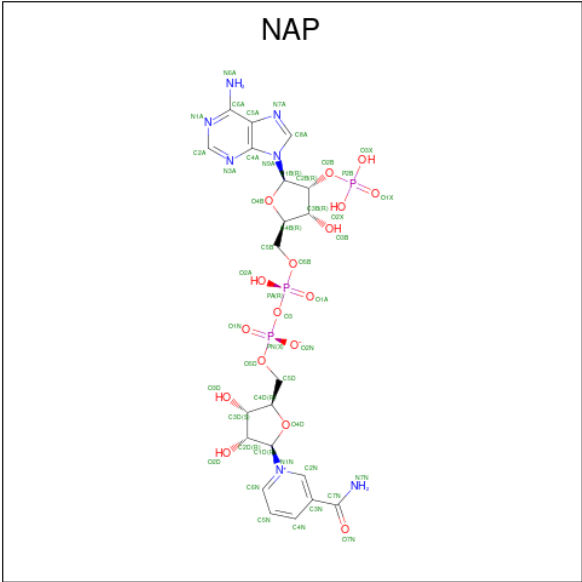
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

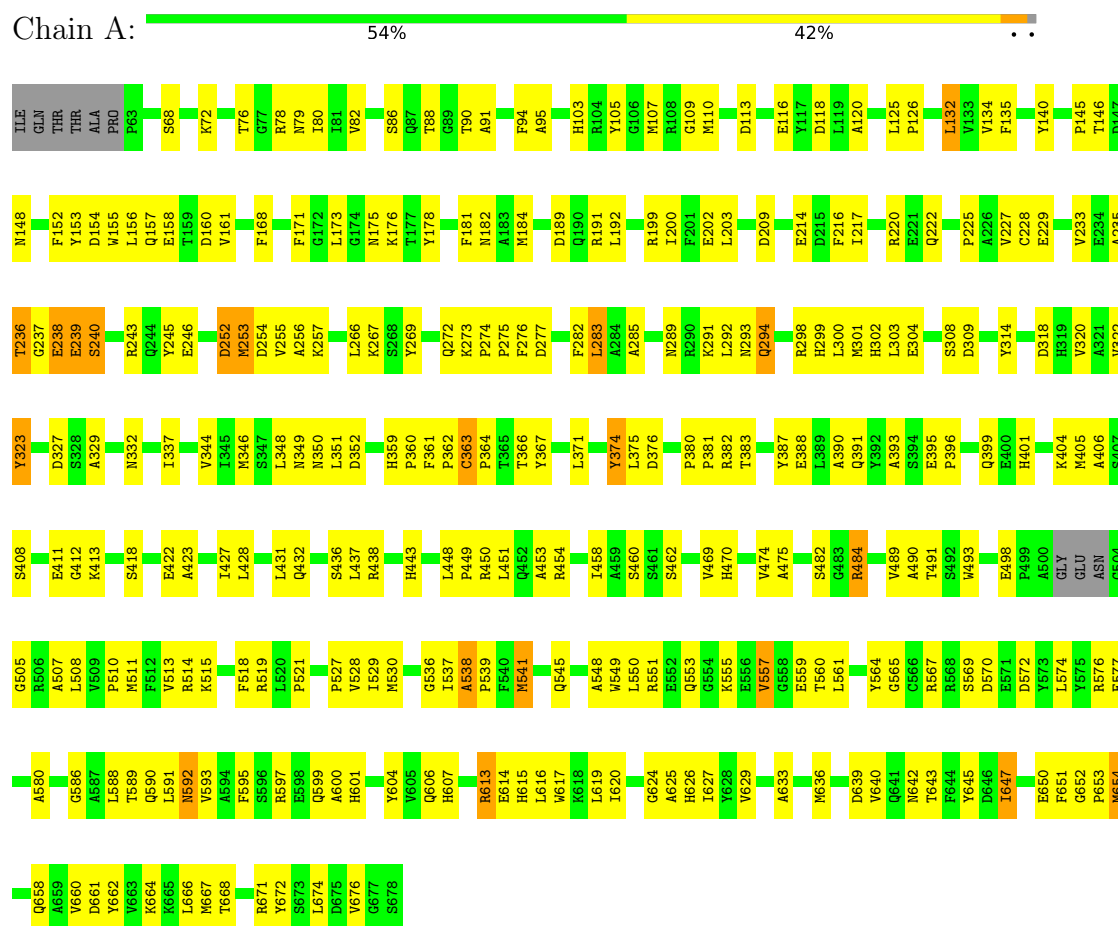
- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



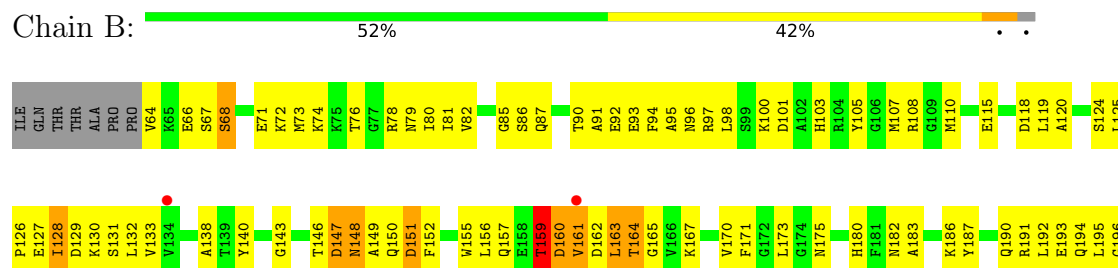
3 Residue-property plots

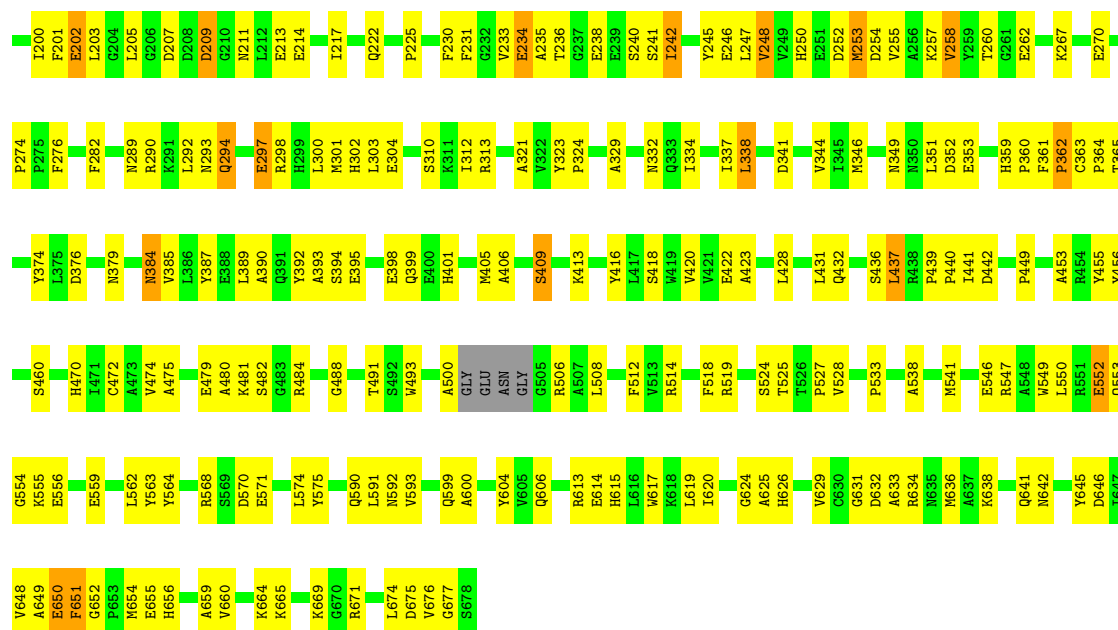
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	101.63Å 116.06Å 118.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	79.6 (30.00-2.70) 79.5 (30.00-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.188 , 0.270 0.187 , 0.267	Depositor DCC
R_{free} test set	1535 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10265	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.35% 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: FMN, FAD, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/5016	0.92	15/6784 (0.2%)
1	B	0.43	0/5004	0.92	15/6768 (0.2%)
All	All	0.45	0/10020	0.92	30/13552 (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 (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	163	LEU	N-CA-C	7.08	117.59	108.24
1	B	479	GLU	N-CA-C	-7.08	99.34	109.96
1	B	297	GLU	N-CA-C	-7.05	102.79	111.33
1	B	553	GLN	N-CA-C	-6.52	105.31	113.20
1	A	363	CYS	N-CA-C	6.25	113.85	108.22
1	B	541	MET	N-CA-C	-6.12	104.72	111.82
1	B	338	LEU	N-CA-C	-5.94	105.52	112.89
1	A	548	ALA	N-CA-C	-5.90	104.77	111.14
1	A	301	MET	N-CA-C	5.84	118.73	109.50
1	A	557	VAL	N-CA-C	5.82	116.24	107.80
1	A	176	LYS	N-CA-C	5.74	119.38	112.38
1	A	647	ILE	N-CA-C	-5.63	105.24	110.53
1	B	143	GLY	N-CA-C	-5.63	106.23	114.90
1	A	202	GLU	N-CA-C	5.44	117.32	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	LYS	CA-C-N	5.43	125.97	120.38
1	A	273	LYS	C-N-CA	5.43	125.97	120.38
1	B	508	LEU	N-CA-C	5.38	119.00	109.96
1	B	290	ARG	N-CA-C	5.36	118.44	110.14
1	B	151	ASP	N-CA-C	-5.33	105.88	112.38
1	B	255	VAL	N-CA-C	5.30	120.36	109.34
1	A	536	GLY	N-CA-C	-5.28	107.77	114.16
1	B	374	TYR	N-CA-C	5.28	120.37	113.30
1	A	160	ASP	N-CA-C	-5.22	105.64	113.89
1	A	541	MET	N-CA-C	-5.22	105.67	111.36
1	B	334	ILE	N-CA-C	-5.21	105.31	110.62
1	A	323	TYR	CA-C-N	5.18	125.65	120.52
1	A	323	TYR	C-N-CA	5.18	125.65	120.52
1	B	209	ASP	N-CA-C	-5.16	106.49	112.89
1	B	258	VAL	N-CA-C	5.13	116.35	108.71
1	A	374	TYR	N-CA-C	5.01	119.67	113.50

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	4901	0	4748	238	0
1	B	4890	0	4737	247	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	31	0	19	4	0
3	B	31	0	19	1	0
4	A	48	0	25	0	0
4	B	48	0	25	3	0
5	A	109	0	0	6	0
5	B	101	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10265	0	9635	483	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 25.

All (483) 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	1.30	1.14
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.33	1.09
1:B:78:ARG:HH22	1:B:352:ASP:HB2	1.26	1.00
1:B:107:MET:HE2	1:B:233:VAL:HG11	1.46	0.97
1:B:163:LEU:HB2	1:B:196:GLY:HA3	1.44	0.96
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.27	0.96
1:B:159:THR:HG22	1:B:161:VAL:H	1.32	0.94
1:A:86:SER:HB3	1:A:91:ALA:HB3	1.48	0.93
1:B:159:THR:HG21	1:B:161:VAL:HG13	1.54	0.90
1:B:665:LYS:HE2	1:B:669:LYS:HE3	1.53	0.90
1:B:167:LYS:HB3	1:B:200:ILE:HD11	1.53	0.88
1:B:159:THR:HG22	1:B:160:ASP:H	1.39	0.88
1:B:78:ARG:NH2	1:B:352:ASP:HB2	1.88	0.88
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.55	0.87
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.36	0.86
1:A:559:GLU:HG2	1:A:589:THR:HG21	1.58	0.86
1:A:350:ASN:HD22	1:A:351:LEU:N	1.75	0.84
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.60	0.83
1:B:294:GLN:H	1:B:294:GLN:NE2	1.75	0.83
1:A:291:LYS:NZ	1:A:293:ASN:HD21	1.77	0.81
1:A:604:TYR:H	1:A:607:HIS:CD2	1.98	0.81
1:A:590:GLN:NE2	1:A:592:ASN:HD21	1.79	0.80
1:B:68:SER:OG	1:B:71:GLU:HG2	1.82	0.78
1:B:568:ARG:NH2	1:B:568:ARG:HB3	1.98	0.78
1:B:78:ARG:HD2	1:B:110:MET:HE3	1.66	0.77
1:A:529:ILE:HD13	1:A:616:LEU:HD22	1.67	0.76
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.67	0.76
1:A:541:MET:O	1:A:545:GLN:HG3	1.86	0.75
1:B:409:SER:HA	1:B:413:LYS:HD3	1.67	0.75
1:A:86:SER:HA	1:A:146:THR:HG21	1.67	0.75
1:A:613:ARG:HD2	1:A:651:PHE:HE1	1.52	0.74
1:A:371:LEU:HD23	1:A:375:LEU:HD12	1.67	0.74
1:B:78:ARG:HD3	1:B:110:MET:HB2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ARG:HG2	1:A:613:ARG:NH1	2.02	0.73
1:B:437:LEU:HD22	1:B:439:PRO:HD3	1.69	0.73
1:A:254:ASP:O	1:A:257:LYS:HG2	1.89	0.72
1:B:159:THR:CG2	1:B:161:VAL:HG13	2.19	0.72
1:B:527:PRO:HB2	1:B:625:ALA:CB	2.14	0.72
1:A:527:PRO:HB2	1:A:625:ALA:CB	2.20	0.71
1:A:214:GLU:OE1	1:A:413:LYS:HE3	1.90	0.71
1:A:549:TRP:O	1:A:553:GLN:HG2	1.91	0.70
1:B:590:GLN:NE2	1:B:592:ASN:HD21	1.89	0.70
1:A:103:HIS:HA	1:A:107:MET:O	1.92	0.69
1:A:135:PHE:CE2	1:A:192:LEU:HD11	2.28	0.69
1:A:521:PRO:HG3	1:A:626:HIS:ND1	2.08	0.69
1:B:533:PRO:HG3	1:B:636:MET:HG3	1.76	0.68
1:A:567:ARG:HD3	1:A:597:ARG:CZ	2.24	0.68
1:B:233:VAL:O	1:B:234:GLU:HG2	1.94	0.67
1:B:323:TYR:CE2	1:B:453:ALA:HB2	2.28	0.67
1:A:86:SER:HB2	3:A:751:FMN:O3P	1.95	0.67
1:A:653:PRO:O	1:A:654:MET:HB3	1.94	0.67
1:B:214:GLU:OE1	1:B:413:LYS:HE3	1.94	0.67
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.77	0.67
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.76	0.66
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.77	0.66
1:B:360:PRO:HG2	1:B:361:PHE:CD1	2.31	0.66
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.78	0.66
1:A:350:ASN:ND2	1:A:352:ASP:H	1.94	0.65
1:A:291:LYS:NZ	1:A:293:ASN:ND2	2.42	0.65
1:B:217:ILE:HD11	1:B:406:ALA:O	1.96	0.65
1:B:568:ARG:HB3	1:B:568:ARG:HH21	1.62	0.65
1:A:590:GLN:HE21	1:A:592:ASN:HD21	1.41	0.65
1:A:246:GLU:HB3	1:A:351:LEU:CD2	2.26	0.64
1:A:217:ILE:HD11	1:A:383:THR:HG21	1.79	0.64
1:A:78:ARG:HD3	1:A:110:MET:HB3	1.80	0.64
1:B:130:LYS:HG3	1:B:231:PHE:HD1	1.61	0.64
1:A:291:LYS:HZ2	1:A:293:ASN:HD21	1.44	0.64
1:A:423:ALA:O	1:A:482:SER:HB3	1.97	0.64
1:B:302:HIS:HD2	1:B:575:TYR:OH	1.81	0.64
1:A:80:ILE:HG23	1:A:109:GLY:HA3	1.80	0.64
1:A:253:MET:HA	1:A:253:MET:HE3	1.80	0.64
1:B:359:HIS:ND1	1:B:363:CYS:HB2	2.14	0.63
1:A:382:ARG:HD2	5:A:760:HOH:O	1.97	0.63
1:A:458:ILE:HG23	1:A:469:VAL:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:HD11	1:B:302:HIS:HB2	1.80	0.63
1:B:656:HIS:O	1:B:660:VAL:HG23	1.98	0.63
1:B:191:ARG:CZ	1:B:195:LEU:HD11	2.29	0.63
1:A:105:TYR:HD1	1:A:235:ALA:HA	1.63	0.62
1:A:615:HIS:O	1:A:619:LEU:HD12	1.98	0.62
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.29	0.62
1:A:344:VAL:O	1:A:366:THR:HG22	1.99	0.62
1:B:617:TRP:HZ3	1:B:648:VAL:HG22	1.64	0.62
1:A:86:SER:HB3	1:A:91:ALA:CB	2.28	0.62
1:A:314:TYR:O	1:A:462:SER:HB3	1.99	0.61
1:A:428:LEU:O	1:A:432:GLN:HG3	2.00	0.61
1:A:266:LEU:O	1:A:267:LYS:HB2	2.00	0.61
1:B:294:GLN:H	1:B:294:GLN:CD	2.08	0.61
1:B:550:LEU:O	1:B:555:LYS:HB2	2.00	0.61
1:B:629:VAL:HB	1:B:674:LEU:HD23	1.81	0.61
1:A:291:LYS:HZ1	1:A:293:ASN:HD21	1.46	0.61
1:A:395:GLU:H	1:A:436:SER:HB2	1.64	0.61
1:A:418:SER:HA	1:A:422:GLU:HB3	1.81	0.61
1:B:203:LEU:HG	1:B:205:LEU:HD21	1.83	0.61
1:B:246:GLU:HB2	1:B:351:LEU:HD21	1.82	0.60
1:A:78:ARG:HH11	1:A:78:ARG:HG3	1.66	0.60
1:A:76:THR:HB	1:A:78:ARG:NH1	2.15	0.60
1:B:167:LYS:HG2	1:B:230:PHE:CE2	2.36	0.60
1:B:214:GLU:O	1:B:217:ILE:HG22	2.01	0.60
1:A:173:LEU:C	1:A:182:ASN:HD21	2.10	0.60
1:A:454:ARG:HH11	1:A:489:VAL:HB	1.66	0.60
1:B:303:LEU:N	1:B:303:LEU:HD12	2.17	0.60
1:B:549:TRP:O	1:B:552:GLU:HG2	2.01	0.60
1:A:300:LEU:N	1:A:300:LEU:HD12	2.17	0.59
1:B:254:ASP:OD1	1:B:257:LYS:HE3	2.01	0.59
1:A:239:GLU:O	1:A:240:SER:HB2	2.02	0.59
1:B:129:ASP:OD1	1:B:130:LYS:HD3	2.02	0.59
1:A:401:HIS:O	1:A:405:MET:HG2	2.03	0.59
1:B:167:LYS:CB	1:B:200:ILE:HD11	2.31	0.59
1:A:551:ARG:HH12	1:A:586:GLY:C	2.10	0.59
1:A:390:ALA:O	1:A:399:GLN:HG3	2.03	0.58
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.68	0.58
1:A:604:TYR:N	1:A:607:HIS:CD2	2.71	0.58
1:B:130:LYS:HG3	1:B:231:PHE:CD1	2.38	0.58
1:A:604:TYR:N	1:A:607:HIS:HD2	2.00	0.58
1:B:68:SER:HG	1:B:71:GLU:HG2	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ALA:O	1:B:146:THR:HG23	2.03	0.58
1:A:189:ASP:HB2	1:A:203:LEU:HD13	1.85	0.58
1:A:591:LEU:HG	1:A:591:LEU:O	2.03	0.58
1:B:276:PHE:CG	1:B:282:PHE:HB2	2.38	0.58
1:B:359:HIS:HB3	1:B:360:PRO:HD2	1.86	0.58
1:A:604:TYR:H	1:A:607:HIS:HD2	1.43	0.58
1:B:528:VAL:HB	1:B:547:ARG:NH1	2.17	0.58
1:B:590:GLN:HE21	1:B:592:ASN:HD21	1.52	0.58
1:A:153:TYR:CE2	1:A:157:GLN:NE2	2.72	0.58
1:A:175:ASN:OD1	1:A:209:ASP:HB2	2.04	0.58
1:B:138:ALA:HA	1:B:173:LEU:HB2	1.85	0.58
1:B:167:LYS:HB3	1:B:200:ILE:CD1	2.30	0.58
1:A:550:LEU:O	1:A:555:LYS:HB2	2.03	0.58
1:B:599:GLN:N	1:B:599:GLN:CD	2.62	0.58
1:A:664:LYS:O	1:A:668:THR:HG23	2.04	0.58
1:B:71:GLU:O	1:B:74:LYS:HB2	2.04	0.57
1:B:180:HIS:HB3	1:B:183:ALA:HB2	1.86	0.57
1:B:293:ASN:ND2	1:B:300:LEU:HD12	2.18	0.57
1:B:301:MET:HE1	1:B:491:THR:O	2.04	0.57
1:B:629:VAL:HB	1:B:674:LEU:CD2	2.34	0.57
1:A:168:PHE:O	1:A:200:ILE:HG22	2.04	0.57
1:B:108:ARG:HG2	1:B:108:ARG:HH21	1.69	0.57
1:B:159:THR:HG22	1:B:160:ASP:N	2.16	0.57
1:A:451:LEU:HD12	5:A:759:HOH:O	2.05	0.56
1:A:662:TYR:HE1	1:A:666:LEU:HD11	1.69	0.56
1:B:125:LEU:N	1:B:126:PRO:HD2	2.21	0.56
1:B:98:LEU:O	1:B:101:ASP:HB2	2.04	0.56
1:B:613:ARG:HG2	1:B:613:ARG:HH11	1.70	0.56
1:A:107:MET:HE1	1:A:227:VAL:HG11	1.87	0.56
1:A:626:HIS:CD2	1:A:671:ARG:HG2	2.41	0.56
1:B:393:ALA:HA	1:B:436:SER:O	2.05	0.56
1:B:133:VAL:O	1:B:133:VAL:HG13	2.05	0.56
1:B:182:ASN:O	1:B:186:LYS:HG3	2.06	0.56
1:A:437:LEU:O	1:A:438:ARG:NH1	2.37	0.56
1:A:428:LEU:HA	1:A:431:LEU:HD12	1.88	0.55
1:A:253:MET:HE2	1:A:257:LYS:HG3	1.89	0.55
1:A:643:THR:O	1:A:647:ILE:HG13	2.05	0.55
1:A:132:LEU:C	1:A:132:LEU:HD12	2.32	0.55
1:B:304:GLU:HG2	1:B:470:HIS:CD2	2.40	0.55
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.88	0.55
1:A:614:GLU:HA	1:A:651:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:HB3	1:B:100:LYS:NZ	2.22	0.55
1:A:561:LEU:HG	1:A:590:GLN:HB2	1.88	0.55
1:A:388:GLU:O	1:A:391:GLN:HG2	2.07	0.54
1:B:186:LYS:O	1:B:190:GLN:HG2	2.06	0.54
1:A:82:VAL:HG11	1:A:95:ALA:HA	1.89	0.54
1:A:624:GLY:HA2	1:A:671:ARG:NH2	2.22	0.54
1:B:247:LEU:HD12	1:B:248:VAL:H	1.73	0.54
1:B:599:GLN:H	1:B:599:GLN:NE2	2.05	0.54
1:B:677:GLY:HA3	4:B:852:NAP:H71N	1.72	0.54
1:A:375:LEU:HD13	1:A:448:LEU:HD12	1.89	0.54
1:A:567:ARG:HD3	1:A:597:ARG:HD2	1.90	0.54
1:A:285:ALA:HA	1:A:508:LEU:HD23	1.90	0.53
1:B:353:GLU:H	1:B:353:GLU:CD	2.16	0.53
1:A:599:GLN:N	1:A:599:GLN:CD	2.66	0.53
1:A:350:ASN:HD22	1:A:351:LEU:H	1.50	0.53
1:A:660:VAL:O	1:A:664:LYS:HG3	2.08	0.53
1:B:93:GLU:O	1:B:97:ARG:HG3	2.08	0.53
1:A:82:VAL:HG22	1:A:134:VAL:HB	1.89	0.53
1:A:560:THR:C	1:A:561:LEU:HD12	2.34	0.53
1:B:514:ARG:HD2	5:B:877:HOH:O	2.08	0.53
1:B:376:ASP:OD2	1:B:379:ASN:ND2	2.42	0.53
1:A:294:GLN:HG3	1:A:570:ASP:HA	1.91	0.53
1:B:107:MET:CE	1:B:233:VAL:HG21	2.39	0.53
1:A:80:ILE:HG23	1:A:109:GLY:CA	2.38	0.53
1:A:645:TYR:CD2	1:A:660:VAL:HA	2.44	0.53
1:B:72:LYS:C	1:B:74:LYS:H	2.17	0.52
1:B:645:TYR:OH	1:B:664:LYS:HE3	2.09	0.52
1:A:591:LEU:O	1:A:593:VAL:HG23	2.09	0.52
1:B:115:GLU:HB2	1:B:148:ASN:O	2.09	0.52
1:A:236:THR:O	1:A:238:GLU:N	2.38	0.52
1:B:398:GLU:O	1:B:401:HIS:HB2	2.08	0.52
1:A:277:ASP:HB2	5:A:860:HOH:O	2.09	0.52
1:B:146:THR:O	1:B:147:ASP:C	2.51	0.52
1:B:519:ARG:HG2	1:B:519:ARG:HH11	1.75	0.52
1:A:460:SER:HB3	1:A:470:HIS:CG	2.45	0.52
1:B:472:CYS:HB3	1:B:538:ALA:HB2	1.91	0.52
1:B:615:HIS:O	1:B:619:LEU:HD13	2.10	0.52
1:B:390:ALA:O	1:B:399:GLN:HG3	2.10	0.52
1:A:274:PRO:HA	1:A:275:PRO:C	2.34	0.52
1:A:475:ALA:HA	1:A:491:THR:HB	1.91	0.52
1:B:289:ASN:OD1	1:B:303:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:HE3	1:A:293:ASN:O	2.09	0.52
1:A:667:MET:HA	1:A:672:TYR:HB3	1.91	0.52
1:A:404:LYS:HG3	1:A:412:GLY:HA3	1.91	0.51
1:B:67:SER:O	1:B:68:SER:C	2.53	0.51
1:B:108:ARG:HG2	1:B:108:ARG:NH2	2.26	0.51
1:B:527:PRO:O	1:B:625:ALA:HB1	2.10	0.51
1:B:97:ARG:CZ	1:B:384:ASN:HB3	2.40	0.51
1:B:236:THR:HG21	1:B:238:GLU:CD	2.36	0.51
1:B:475:ALA:HA	1:B:491:THR:HB	1.91	0.51
1:A:276:PHE:CG	1:A:282:PHE:HB2	2.46	0.51
1:A:371:LEU:HD23	1:A:375:LEU:CD1	2.37	0.51
1:B:258:VAL:CG1	1:B:365:THR:HA	2.41	0.51
1:B:167:LYS:HG2	1:B:230:PHE:HE2	1.75	0.51
1:B:167:LYS:HD2	1:B:167:LYS:N	2.26	0.51
1:B:170:VAL:HG12	1:B:171:PHE:N	2.25	0.51
1:B:233:VAL:C	1:B:235:ALA:H	2.18	0.51
1:B:159:THR:HG22	1:B:161:VAL:N	2.14	0.51
1:B:626:HIS:CD2	1:B:671:ARG:HG2	2.46	0.51
1:B:428:LEU:O	1:B:432:GLN:HG3	2.11	0.50
1:A:228:CYS:HA	1:A:233:VAL:CG2	2.41	0.50
1:A:654:MET:HB2	1:A:658:GLN:HB2	1.92	0.50
1:A:511:MET:SD	1:A:511:MET:C	2.94	0.50
1:B:86:SER:HB2	1:B:91:ALA:CB	2.21	0.50
1:B:392:TYR:CD1	1:B:440:PRO:HD3	2.46	0.50
1:A:291:LYS:HZ1	1:A:293:ASN:ND2	2.05	0.50
1:A:427:ILE:HG23	1:A:428:LEU:N	2.27	0.50
1:B:546:GLU:O	1:B:549:TRP:HB3	2.12	0.50
1:A:567:ARG:HD3	1:A:597:ARG:NE	2.26	0.50
1:A:636:MET:O	1:A:640:VAL:HG23	2.12	0.50
1:B:132:LEU:H	1:B:132:LEU:HD23	1.75	0.50
1:B:376:ASP:CB	1:B:449:PRO:HG2	2.41	0.50
1:B:528:VAL:HB	1:B:547:ARG:HH11	1.77	0.50
1:A:272:GLN:OE1	1:A:282:PHE:HA	2.12	0.49
1:A:346:MET:HG2	1:A:367:TYR:CZ	2.47	0.49
1:B:222:GLN:C	1:B:225:PRO:HD2	2.37	0.49
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.94	0.49
1:B:81:ILE:HG13	1:B:110:MET:O	2.12	0.49
1:A:454:ARG:NH1	1:A:489:VAL:HB	2.27	0.49
1:A:222:GLN:O	1:A:225:PRO:HD2	2.12	0.49
1:A:152:PHE:CZ	1:A:156:LEU:HD11	2.47	0.49
1:A:318:ASP:OD1	1:A:515:LYS:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ASN:O	1:A:645:TYR:N	2.46	0.49
1:B:418:SER:HA	1:B:422:GLU:HB3	1.94	0.49
1:A:304:GLU:HG2	1:A:470:HIS:CD2	2.48	0.49
1:B:73:MET:HB2	1:B:78:ARG:O	2.12	0.49
1:A:561:LEU:HD12	1:A:561:LEU:N	2.27	0.49
1:A:650:GLU:OE1	1:A:651:PHE:CE1	2.66	0.48
1:A:269:TYR:HB2	5:A:825:HOH:O	2.12	0.48
1:A:559:GLU:OE1	1:A:619:LEU:HD21	2.13	0.48
1:B:78:ARG:CD	1:B:110:MET:HB2	2.42	0.48
1:A:361:PHE:HB2	1:A:362:PRO:HD2	1.94	0.48
1:B:162:ASP:OD1	1:B:163:LEU:N	2.47	0.48
1:B:175:ASN:HA	1:B:207:ASP:OD1	2.14	0.48
1:A:624:GLY:C	1:A:671:ARG:NH2	2.72	0.48
1:B:297:GLU:HG3	1:B:571:GLU:OE1	2.13	0.48
1:B:159:THR:O	1:B:160:ASP:HB2	2.12	0.48
1:A:337:ILE:HB	1:B:600:ALA:HB1	1.95	0.48
1:B:423:ALA:HA	1:B:481:LYS:HB2	1.95	0.48
1:B:617:TRP:CZ3	1:B:648:VAL:HG22	2.46	0.48
1:B:293:ASN:ND2	1:B:298:ARG:O	2.46	0.48
1:B:341:ASP:HB3	1:B:344:VAL:HG23	1.96	0.48
1:B:631:GLY:N	1:B:676:VAL:HG12	2.28	0.48
1:A:350:ASN:HD22	1:A:350:ASN:C	2.17	0.48
1:B:79:ASN:ND2	1:B:80:ILE:HG13	2.28	0.48
1:B:310:SER:C	1:B:312:ILE:H	2.21	0.48
1:B:624:GLY:C	1:B:671:ARG:HH21	2.22	0.48
1:A:427:ILE:HG23	1:A:428:LEU:H	1.79	0.47
1:B:231:PHE:HB2	1:B:233:VAL:HG23	1.96	0.47
1:B:360:PRO:HG2	1:B:361:PHE:CE1	2.49	0.47
1:A:243:ARG:NH2	1:A:443:HIS:HA	2.29	0.47
1:B:677:GLY:HA3	4:B:852:NAP:N7N	2.29	0.47
1:B:236:THR:CG2	1:B:238:GLU:HG2	2.43	0.47
1:B:552:GLU:HG2	1:B:552:GLU:H	1.56	0.47
1:A:653:PRO:O	1:A:654:MET:CB	2.61	0.47
1:B:90:THR:HG22	1:B:94:PHE:CE2	2.49	0.47
1:B:641:GLN:NE2	1:B:645:TYR:OH	2.39	0.47
1:A:569:SER:HB3	1:A:595:PHE:CE1	2.48	0.47
1:B:191:ARG:HD3	1:B:195:LEU:HD13	1.97	0.47
1:A:349:ASN:OD1	1:A:359:HIS:HE1	1.97	0.47
1:A:395:GLU:OE2	1:A:396:PRO:HD2	2.15	0.47
1:A:625:ALA:N	1:A:671:ARG:HH21	2.12	0.47
1:B:128:ILE:HG22	1:B:131:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:VAL:O	1:A:474:VAL:HG13	2.14	0.47
1:B:163:LEU:HG	1:B:164:THR:OG1	2.15	0.47
1:B:654:MET:SD	1:B:659:ALA:HA	2.54	0.47
1:A:408:SER:O	1:A:413:LYS:HD2	2.15	0.47
1:A:528:VAL:HG12	1:A:530:MET:HG3	1.97	0.47
1:A:569:SER:O	1:A:576:ARG:NH1	2.46	0.47
1:A:662:TYR:CD1	1:A:662:TYR:C	2.92	0.47
1:B:233:VAL:O	1:B:235:ALA:N	2.48	0.47
1:B:294:GLN:CD	1:B:294:GLN:N	2.71	0.47
1:B:646:ASP:HA	1:B:649:ALA:HB3	1.97	0.47
1:B:140:TYR:CD2	1:B:146:THR:HG22	2.50	0.47
1:B:247:LEU:HD11	1:B:346:MET:HB2	1.97	0.47
1:B:292:LEU:CD1	1:B:302:HIS:HB2	2.43	0.47
1:B:338:LEU:CD2	1:B:439:PRO:HD2	2.45	0.47
1:B:201:PHE:O	1:B:202:GLU:O	2.33	0.46
1:A:292:LEU:HD11	1:A:302:HIS:HB2	1.97	0.46
1:A:361:PHE:HB2	1:A:362:PRO:CD	2.46	0.46
1:B:159:THR:HG23	1:B:191:ARG:NH2	2.30	0.46
1:A:236:THR:O	1:A:236:THR:HG22	2.14	0.46
1:B:124:SER:O	1:B:127:GLU:HB2	2.16	0.46
1:B:209:ASP:OD1	1:B:634:ARG:NH2	2.47	0.46
1:A:253:MET:HE2	1:A:257:LYS:CG	2.45	0.46
1:B:85:GLY:O	1:B:138:ALA:HB3	2.14	0.46
1:B:274:PRO:HG3	1:B:276:PHE:CE2	2.50	0.46
1:B:245:TYR:HA	1:B:349:ASN:O	2.15	0.46
1:A:308:SER:O	1:A:309:ASP:HB2	2.16	0.46
1:B:147:ASP:O	1:B:149:ALA:N	2.49	0.46
1:A:564:TYR:CG	1:A:565:GLY:N	2.84	0.46
1:B:651:PHE:HD1	1:B:651:PHE:H	1.64	0.46
1:A:86:SER:CA	1:A:146:THR:HG21	2.44	0.46
1:A:105:TYR:CD1	1:A:235:ALA:HA	2.48	0.46
1:A:323:TYR:CE2	1:A:453:ALA:HB2	2.51	0.46
1:B:97:ARG:NH1	1:B:213:GLU:OE1	2.46	0.46
1:B:214:GLU:CD	1:B:413:LYS:HE3	2.40	0.46
1:B:301:MET:HG3	1:B:303:LEU:HD11	1.98	0.46
1:B:392:TYR:CE1	1:B:440:PRO:HD3	2.51	0.46
1:B:480:ALA:C	1:B:482:SER:H	2.24	0.46
1:A:298:ARG:HD2	5:A:773:HOH:O	2.16	0.46
1:B:76:THR:OG1	1:B:78:ARG:HG3	2.16	0.46
1:B:85:GLY:O	1:B:146:THR:HG21	2.16	0.46
1:B:252:ASP:O	1:B:253:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASP:HB3	1:A:116:GLU:HG3	1.98	0.46
1:A:322:VAL:O	1:A:453:ALA:HA	2.16	0.46
1:A:538:ALA:HB3	1:A:539:PRO:CD	2.46	0.46
1:A:567:ARG:HD3	1:A:597:ARG:CD	2.46	0.45
1:A:577:GLU:O	1:A:580:ALA:HB3	2.15	0.45
1:B:80:ILE:HG12	1:B:132:LEU:HD23	1.97	0.45
1:B:240:SER:O	1:B:242:ILE:N	2.49	0.45
1:A:567:ARG:HD3	1:A:597:ARG:NH1	2.31	0.45
1:B:118:ASP:C	1:B:120:ALA:H	2.24	0.45
1:B:432:GLN:OE1	1:B:484:ARG:NH1	2.48	0.45
1:A:118:ASP:C	1:A:120:ALA:H	2.25	0.45
1:A:289:ASN:ND2	1:A:303:LEU:HG	2.31	0.45
1:A:588:LEU:HD13	1:A:591:LEU:HD13	1.99	0.45
1:B:321:ALA:HB3	1:B:512:PHE:CE1	2.52	0.45
1:B:416:TYR:O	1:B:420:VAL:HB	2.17	0.45
1:A:332:ASN:N	1:A:332:ASN:HD22	2.14	0.45
1:A:633:ALA:HB2	1:A:676:VAL:CB	2.42	0.45
1:B:73:MET:HB2	1:B:78:ARG:HB2	1.98	0.45
1:B:346:MET:HE3	1:B:365:THR:O	2.17	0.45
1:A:393:ALA:HA	1:A:436:SER:O	2.16	0.45
1:A:606:GLN:HE21	1:A:639:ASP:HB3	1.82	0.45
1:B:191:ARG:O	1:B:194:GLN:HB2	2.16	0.45
1:B:632:ASP:OD2	1:B:633:ALA:N	2.49	0.45
1:A:153:TYR:O	1:A:154:ASP:C	2.60	0.45
1:A:454:ARG:HG3	1:A:490:ALA:CB	2.46	0.45
1:A:513:VAL:HG12	1:A:514:ARG:N	2.31	0.45
1:A:484:ARG:N	1:A:484:ARG:HD2	2.31	0.45
1:A:493:TRP:HH2	1:A:510:PRO:HD2	1.82	0.45
1:B:151:ASP:O	1:B:155:TRP:HB2	2.16	0.45
1:B:170:VAL:HB	1:B:203:LEU:HD13	1.98	0.45
1:A:78:ARG:NH2	1:A:352:ASP:OD1	2.50	0.44
1:A:88:THR:OG1	3:A:751:FMN:O1P	2.33	0.44
1:A:299:HIS:C	1:A:300:LEU:HD12	2.42	0.44
1:A:404:LYS:HE3	5:A:805:HOH:O	2.16	0.44
1:A:551:ARG:NH1	1:A:586:GLY:C	2.75	0.44
1:B:164:THR:HG22	1:B:165:GLY:N	2.32	0.44
1:A:482:SER:OG	1:A:484:ARG:HD3	2.17	0.44
1:B:568:ARG:HH21	1:B:568:ARG:CB	2.27	0.44
1:A:283:LEU:HB3	1:A:508:LEU:HD13	1.99	0.44
1:A:291:LYS:HZ2	1:A:293:ASN:ND2	2.08	0.44
1:A:551:ARG:C	1:A:553:GLN:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LEU:HD21	1:B:439:PRO:HD2	1.99	0.44
1:A:222:GLN:C	1:A:225:PRO:HD2	2.42	0.44
1:A:363:CYS:HB3	1:A:364:PRO:HA	1.98	0.44
1:A:514:ARG:HG3	1:A:514:ARG:NH1	2.30	0.44
1:B:203:LEU:HG	1:B:205:LEU:CD2	2.47	0.44
1:B:203:LEU:CG	1:B:205:LEU:HD21	2.48	0.44
1:B:518:PHE:CE2	1:B:675:ASP:HB2	2.52	0.44
1:B:650:GLU:C	1:B:652:GLY:H	2.26	0.44
1:A:617:TRP:CH2	1:A:652:GLY:HA2	2.53	0.44
1:A:624:GLY:HA2	1:A:671:ARG:CZ	2.48	0.44
1:B:401:HIS:O	1:B:405:MET:HG2	2.18	0.44
1:B:431:LEU:HD23	1:B:437:LEU:HD13	1.99	0.44
1:B:633:ALA:O	1:B:638:LYS:HE2	2.18	0.44
1:B:599:GLN:N	1:B:599:GLN:NE2	2.66	0.44
1:B:614:GLU:HB2	5:B:875:HOH:O	2.18	0.44
1:A:140:TYR:CE1	1:A:146:THR:HG22	2.53	0.44
1:A:171:PHE:C	1:A:171:PHE:CD2	2.96	0.44
1:A:181:PHE:O	1:A:182:ASN:HB2	2.17	0.44
1:A:252:ASP:O	1:A:253:MET:C	2.61	0.44
1:B:163:LEU:N	1:B:163:LEU:HD23	2.33	0.44
1:B:361:PHE:O	1:B:362:PRO:C	2.61	0.44
1:B:488:GLY:HA3	2:B:850:FAD:O2P	2.17	0.44
1:B:207:ASP:OD2	1:B:209:ASP:HB3	2.18	0.43
1:B:441:ILE:HG23	1:B:442:ASP:N	2.33	0.43
1:B:519:ARG:HG2	1:B:519:ARG:NH1	2.33	0.43
1:A:645:TYR:CE2	1:A:660:VAL:HA	2.52	0.43
1:B:234:GLU:O	1:B:235:ALA:HB3	2.18	0.43
1:A:155:TRP:CE3	1:A:156:LEU:HD23	2.52	0.43
1:A:228:CYS:SG	1:A:233:VAL:HG23	2.58	0.43
1:A:600:ALA:HB1	1:B:337:ILE:HB	2.00	0.43
1:B:207:ASP:CG	1:B:209:ASP:H	2.27	0.43
1:B:248:VAL:HG12	1:B:250:HIS:CD2	2.53	0.43
1:B:387:TYR:CD1	1:B:387:TYR:C	2.97	0.43
1:B:156:LEU:HB2	1:B:187:TYR:HE2	1.83	0.43
1:B:525:THR:HG22	1:B:556:GLU:O	2.19	0.43
1:B:660:VAL:HG12	1:B:664:LYS:HD3	2.01	0.43
1:A:86:SER:CB	3:A:751:FMN:O3P	2.66	0.43
1:B:157:GLN:C	1:B:159:THR:H	2.27	0.43
1:B:329:ALA:HA	1:B:332:ASN:HD22	1.82	0.43
1:A:175:ASN:HB3	1:A:178:TYR:HD2	1.83	0.43
1:B:92:GLU:HG2	1:B:96:ASN:HD21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PRO:HB3	1:B:165:GLY:C	2.43	0.43
1:B:150:GLN:C	1:B:152:PHE:N	2.74	0.43
1:A:145:PRO:HA	1:A:184:MET:HG3	2.01	0.43
1:A:454:ARG:HG3	1:A:490:ALA:HB3	2.00	0.43
1:A:460:SER:HB3	1:A:470:HIS:ND1	2.32	0.43
1:A:348:LEU:HB2	1:A:360:PRO:CD	2.49	0.43
1:B:409:SER:HA	1:B:413:LYS:CD	2.44	0.43
1:B:564:TYR:O	1:B:593:VAL:HA	2.19	0.43
1:B:606:GLN:OE1	4:B:852:NAP:H2A	2.19	0.43
1:A:374:TYR:O	1:A:450:ARG:HD2	2.18	0.43
1:B:82:VAL:HG11	1:B:95:ALA:HA	2.00	0.43
1:B:562:LEU:HD12	1:B:563:TYR:H	1.84	0.43
1:A:72:LYS:HE3	1:A:72:LYS:HB2	1.63	0.42
1:A:86:SER:H	1:A:148:ASN:HD21	1.67	0.42
1:A:344:VAL:C	1:A:366:THR:HG22	2.44	0.42
1:A:599:GLN:HG2	1:A:601:HIS:O	2.19	0.42
1:B:385:VAL:O	1:B:389:LEU:HG	2.19	0.42
1:B:103:HIS:C	1:B:105:TYR:H	2.27	0.42
1:B:193:GLU:C	1:B:195:LEU:N	2.76	0.42
1:B:385:VAL:HG12	1:B:389:LEU:HD12	2.01	0.42
1:A:245:TYR:CD1	1:A:360:PRO:HD3	2.54	0.42
1:A:551:ARG:NH1	1:A:586:GLY:O	2.52	0.42
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.84	0.42
1:B:568:ARG:NH2	1:B:570:ASP:CG	2.78	0.42
1:A:107:MET:HE1	1:A:227:VAL:CG1	2.49	0.42
1:A:235:ALA:O	1:A:238:GLU:HG3	2.20	0.42
1:A:266:LEU:O	1:A:267:LYS:CB	2.66	0.42
1:B:274:PRO:HG3	1:B:276:PHE:HE2	1.84	0.42
1:B:302:HIS:CD2	1:B:575:TYR:OH	2.65	0.42
1:A:79:ASN:HD21	1:A:107:MET:HB3	1.85	0.42
1:A:135:PHE:HE2	1:A:192:LEU:HD11	1.77	0.42
1:A:537:ILE:O	1:A:538:ALA:C	2.63	0.42
1:A:567:ARG:CG	1:A:567:ARG:HH11	2.32	0.42
1:B:72:LYS:C	1:B:74:LYS:N	2.77	0.42
1:B:191:ARG:O	1:B:192:LEU:C	2.60	0.42
1:B:651:PHE:N	1:B:651:PHE:CD1	2.88	0.42
1:A:661:ASP:O	1:A:662:TYR:C	2.61	0.42
1:B:267:LYS:HE3	1:B:270:GLU:OE1	2.20	0.42
1:A:613:ARG:HH11	1:A:613:ARG:CG	2.16	0.42
1:A:619:LEU:HD12	1:A:619:LEU:H	1.85	0.42
1:A:553:GLN:HA	1:A:553:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:O	1:A:76:THR:HG23	2.20	0.41
1:B:474:VAL:O	1:B:474:VAL:HG13	2.20	0.41
1:A:125:LEU:N	1:A:126:PRO:CD	2.83	0.41
1:A:238:GLU:O	1:A:239:GLU:HB2	2.20	0.41
1:A:327:ASP:OD1	1:A:329:ALA:HB3	2.20	0.41
1:B:214:GLU:HA	1:B:217:ILE:HG22	2.02	0.41
1:B:500:ALA:O	1:B:506:ARG:HB3	2.20	0.41
1:A:78:ARG:HG3	1:A:78:ARG:NH1	2.33	0.41
1:A:189:ASP:OD2	1:A:199:ARG:HD3	2.20	0.41
1:A:380:PRO:HA	1:A:381:PRO:HD3	1.93	0.41
1:B:140:TYR:HE2	3:B:851:FMN:O2P	2.03	0.41
1:B:604:TYR:HB3	1:B:606:GLN:OE1	2.19	0.41
1:A:94:PHE:HB3	1:A:216:PHE:CE1	2.56	0.41
1:A:599:GLN:N	1:A:599:GLN:OE1	2.54	0.41
1:B:562:LEU:HD12	1:B:563:TYR:N	2.36	0.41
1:B:87:GLN:HB2	1:B:140:TYR:CZ	2.56	0.41
1:B:233:VAL:C	1:B:235:ALA:N	2.79	0.41
1:B:80:ILE:HG12	1:B:132:LEU:CD2	2.50	0.41
1:B:559:GLU:OE2	1:B:619:LEU:HD21	2.20	0.41
1:A:90:THR:HG22	1:A:173:LEU:HD21	2.02	0.41
1:A:498:GLU:O	1:A:507:ALA:HB2	2.21	0.41
1:B:527:PRO:O	1:B:625:ALA:CB	2.69	0.41
1:A:140:TYR:OH	3:A:751:FMN:O2P	2.37	0.41
1:B:323:TYR:CD2	1:B:453:ALA:HB2	2.56	0.41
1:B:363:CYS:HA	1:B:364:PRO:C	2.46	0.41
1:B:394:SER:O	1:B:395:GLU:C	2.63	0.41
1:B:460:SER:HB3	1:B:470:HIS:CG	2.56	0.41
1:A:300:LEU:HD22	1:A:574:LEU:HD21	2.03	0.41
1:A:383:THR:HB	1:A:406:ALA:HB2	2.03	0.41
1:B:138:ALA:HB2	1:B:173:LEU:HD22	2.02	0.40
1:B:564:TYR:OH	1:B:574:LEU:HG	2.20	0.40
1:A:255:VAL:C	1:A:257:LYS:H	2.29	0.40
1:B:324:PRO:HA	1:B:493:TRP:CD2	2.56	0.40
1:A:78:ARG:CD	1:A:110:MET:HB3	2.50	0.40
1:A:239:GLU:CD	1:A:387:TYR:OH	2.64	0.40
1:A:518:PHE:O	1:A:519:ARG:HG2	2.22	0.40
1:A:620:ILE:CD1	1:A:627:ILE:HD11	2.51	0.40
1:B:321:ALA:HB2	1:B:455:TYR:CE1	2.56	0.40
1:B:552:GLU:C	1:B:554:GLY:H	2.28	0.40
1:B:642:ASN:HA	1:B:645:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	609/622 (98%)	536 (88%)	61 (10%)	12 (2%)	6	16
1	B	607/622 (98%)	516 (85%)	69 (11%)	22 (4%)	2	6
All	All	1216/1244 (98%)	1052 (86%)	130 (11%)	34 (3%)	4	9

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	GLU
1	B	159	THR
1	B	160	ASP
1	B	202	GLU
1	B	234	GLU
1	B	241	SER
1	A	236	THR
1	A	237	GLY
1	A	654	MET
1	B	68	SER
1	B	148	ASN
1	B	164	THR
1	B	409	SER
1	B	524	SER
1	B	651	PHE
1	A	253	MET
1	A	256	ALA
1	B	147	ASP
1	B	253	MET
1	A	68	SER
1	A	238	GLU
1	A	240	SER
1	A	505	GLY
1	B	119	LEU
1	B	211	ASN

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Mol	Chain	Res	Type
1	B	620	ILE
1	B	655	GLU
1	A	538	ALA
1	A	592	ASN
1	B	161	VAL
1	B	650	GLU
1	A	161	VAL
1	B	362	PRO
1	B	248	VAL

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	523/530 (99%)	510 (98%)	13 (2%)	42	71
1	B	522/530 (98%)	511 (98%)	11 (2%)	47	75
All	All	1045/1060 (99%)	1021 (98%)	24 (2%)	44	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	158	GLU
1	A	220	ARG
1	A	229	GLU
1	A	239	GLU
1	A	252	ASP
1	A	283	LEU
1	A	294	GLN
1	A	320	VAL
1	A	411	GLU
1	A	484	ARG
1	A	572	ASP
1	A	613	ARG
1	B	64	VAL

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Mol	Chain	Res	Type
1	B	128	ILE
1	B	159	THR
1	B	242	ILE
1	B	260	THR
1	B	262	GLU
1	B	294	GLN
1	B	384	ASN
1	B	437	LEU
1	B	552	GLU
1	B	591	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	150	GLN
1	A	157	GLN
1	A	182	ASN
1	A	190	GLN
1	A	289	ASN
1	A	293	ASN
1	A	332	ASN
1	A	350	ASN
1	A	356	ASN
1	A	359	HIS
1	A	384	ASN
1	A	391	GLN
1	A	399	GLN
1	A	401	HIS
1	A	452	GLN
1	A	465	HIS
1	A	467	ASN
1	A	470	HIS
1	A	486	ASN
1	A	553	GLN
1	A	583	HIS
1	A	590	GLN
1	A	607	HIS
1	B	87	GLN
1	B	96	ASN
1	B	148	ASN
1	B	180	HIS

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Mol	Chain	Res	Type
1	B	182	ASN
1	B	271	ASN
1	B	272	GLN
1	B	294	GLN
1	B	302	HIS
1	B	332	ASN
1	B	333	GLN
1	B	349	ASN
1	B	399	GLN
1	B	467	ASN
1	B	486	ASN
1	B	517	GLN
1	B	590	GLN
1	B	599	GLN
1	B	635	ASN

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMN	A	751	-	33,33,33	2.21	12 (36%)	48,50,50	1.53	8 (16%)
2	FAD	B	850	-	58,58,58	2.65	21 (36%)	85,89,89	1.37	12 (14%)
3	FMN	B	851	-	33,33,33	2.45	12 (36%)	48,50,50	1.69	10 (20%)
4	NAP	A	752	-	50,52,52	4.16	21 (42%)	71,80,80	1.47	12 (16%)
4	NAP	B	852	-	50,52,52	4.15	18 (36%)	71,80,80	1.47	12 (16%)
2	FAD	A	750	-	58,58,58	2.64	23 (39%)	85,89,89	1.36	12 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	A	751	-	-	0/18/18/18	0/3/3/3
2	FAD	B	850	-	-	2/34/50/50	0/6/6/6
3	FMN	B	851	-	-	0/18/18/18	0/3/3/3
4	NAP	A	752	-	-	5/35/67/67	0/5/5/5
4	NAP	B	852	-	-	9/35/67/67	0/5/5/5
2	FAD	A	750	-	-	3/34/50/50	0/6/6/6

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	752	NAP	C2N-N1N	15.61	1.52	1.35
4	B	852	NAP	C2N-N1N	15.38	1.51	1.35
4	B	852	NAP	C4N-C3N	11.94	1.57	1.39
4	A	752	NAP	C4N-C3N	11.35	1.56	1.39
4	B	852	NAP	PN-O3	-9.10	1.49	1.59
4	A	752	NAP	PA-O3	-8.88	1.49	1.59
4	B	852	NAP	PA-O3	-8.47	1.50	1.59
4	A	752	NAP	PN-O3	-8.43	1.50	1.59
4	A	752	NAP	C4A-N3A	8.42	1.50	1.34
4	B	852	NAP	C4A-N3A	7.65	1.48	1.34
4	A	752	NAP	C6N-C5N	7.17	1.53	1.38
4	B	852	NAP	C6N-C5N	7.00	1.53	1.38
4	A	752	NAP	C7N-N7N	6.93	1.45	1.33
2	B	850	FAD	C10-N10	6.47	1.51	1.37
3	B	851	FMN	C10-N10	6.46	1.51	1.37
4	B	852	NAP	C7N-N7N	6.41	1.44	1.33
2	B	850	FAD	P-O3P	-6.18	1.52	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	FAD	C9A-C5X	5.92	1.50	1.41
2	A	750	FAD	C4A-N3A	5.65	1.45	1.34
2	A	750	FAD	C10-N10	5.63	1.49	1.37
2	B	850	FAD	C1'-C2'	5.57	1.60	1.52
2	B	850	FAD	C5'-C4'	-5.43	1.44	1.51
2	A	750	FAD	C4X-N5	5.37	1.42	1.30
3	A	751	FMN	C10-N10	5.30	1.48	1.37
4	B	852	NAP	P2B-O2B	-5.29	1.50	1.59
4	A	752	NAP	P2B-O2B	-5.26	1.50	1.59
4	B	852	NAP	C2A-N1A	5.20	1.43	1.33
4	A	752	NAP	C2A-N1A	5.20	1.43	1.33
2	B	850	FAD	C4A-N3A	5.15	1.44	1.34
3	A	751	FMN	C4A-N5	5.12	1.41	1.30
3	B	851	FMN	C9-C9A	5.10	1.47	1.39
2	B	850	FAD	C9A-N10	4.83	1.49	1.41
2	A	750	FAD	C5'-C4'	-4.74	1.45	1.51
4	B	852	NAP	C5A-C6A	4.73	1.54	1.41
3	B	851	FMN	C9A-N10	4.73	1.49	1.41
4	A	752	NAP	C5A-C6A	4.68	1.54	1.41
2	B	850	FAD	C4X-N5	4.66	1.40	1.30
2	A	750	FAD	C9A-N10	4.64	1.49	1.41
2	A	750	FAD	P-O3P	-4.63	1.54	1.59
2	B	850	FAD	C9A-C5X	4.54	1.48	1.41
2	B	850	FAD	PA-O3P	-4.35	1.54	1.59
3	B	851	FMN	C4A-N5	4.32	1.40	1.30
3	A	751	FMN	C9-C9A	4.31	1.46	1.39
2	A	750	FAD	C2'-C3'	4.27	1.60	1.53
2	A	750	FAD	C6-C5X	4.23	1.46	1.40
2	A	750	FAD	C6-C7	4.17	1.45	1.39
2	B	850	FAD	C9-C9A	4.15	1.46	1.39
2	A	750	FAD	C8-C7	4.02	1.50	1.40
3	B	851	FMN	C9A-C5A	4.01	1.47	1.41
3	A	751	FMN	C9A-N10	4.00	1.48	1.41
2	A	750	FAD	C8A-N7A	3.91	1.39	1.31
2	B	850	FAD	C6-C5X	3.83	1.45	1.40
3	B	851	FMN	C8-C7	3.79	1.50	1.40
2	B	850	FAD	C8-C7	3.57	1.49	1.40
3	B	851	FMN	C10-N1	3.57	1.40	1.33
2	A	750	FAD	C9-C9A	3.49	1.45	1.39
2	A	750	FAD	PA-O5B	-3.38	1.46	1.59
3	A	751	FMN	C9A-C5A	3.30	1.46	1.41
2	A	750	FAD	PA-O3P	-3.28	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	852	NAP	PN-O5D	-3.25	1.46	1.59
2	A	750	FAD	C5A-C4A	3.25	1.44	1.39
4	A	752	NAP	C4A-N9A	-3.23	1.31	1.37
4	B	852	NAP	PA-O5B	-3.23	1.46	1.59
3	A	751	FMN	C8-C7	3.23	1.48	1.40
2	B	850	FAD	C2'-C3'	3.20	1.59	1.53
2	B	850	FAD	PA-O5B	-3.19	1.46	1.59
3	B	851	FMN	C4'-C3'	3.09	1.58	1.53
4	B	852	NAP	C4A-N9A	-3.08	1.31	1.37
2	B	850	FAD	C6-C7	3.03	1.43	1.39
2	B	850	FAD	C8A-N7A	2.95	1.37	1.31
4	A	752	NAP	PA-O5B	-2.94	1.47	1.59
2	B	850	FAD	C2A-N3A	2.93	1.39	1.33
2	A	750	FAD	C2A-N1A	2.89	1.39	1.33
4	A	752	NAP	PN-O5D	-2.87	1.48	1.59
3	A	751	FMN	C6-C5A	2.87	1.44	1.40
4	B	852	NAP	C3N-C7N	2.80	1.54	1.50
3	A	751	FMN	C10-N1	2.80	1.38	1.33
4	A	752	NAP	C6A-N6A	-2.68	1.27	1.34
2	B	850	FAD	C10-N1	2.67	1.38	1.33
4	A	752	NAP	C3N-C7N	2.54	1.54	1.50
4	B	852	NAP	C5A-N7A	2.49	1.43	1.39
4	A	752	NAP	C5D-C4D	2.48	1.59	1.51
4	B	852	NAP	C5D-C4D	2.44	1.58	1.51
4	B	852	NAP	C6A-N6A	-2.44	1.28	1.34
2	A	750	FAD	C8A-N9A	2.44	1.41	1.37
3	A	751	FMN	P-O3P	-2.44	1.45	1.54
3	B	851	FMN	C6-C5A	2.43	1.43	1.40
2	A	750	FAD	C1'-C2'	2.40	1.56	1.52
2	A	750	FAD	C10-N1	2.37	1.38	1.33
3	B	851	FMN	P-O3P	-2.34	1.46	1.54
3	B	851	FMN	C8M-C8	2.33	1.55	1.51
4	A	752	NAP	C5A-N7A	2.33	1.43	1.39
3	A	751	FMN	C4'-C3'	2.33	1.57	1.53
2	B	850	FAD	C1B-N9A	2.30	1.52	1.46
2	A	750	FAD	C1B-N9A	2.25	1.52	1.46
2	A	750	FAD	C7M-C7	2.17	1.55	1.51
3	B	851	FMN	P-O2P	-2.17	1.46	1.54
4	B	852	NAP	P2B-O2X	-2.17	1.46	1.54
4	A	752	NAP	P2B-O3X	-2.11	1.47	1.54
2	A	750	FAD	C6A-N1A	2.11	1.41	1.35
4	A	752	NAP	O4D-C1D	2.10	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	850	FAD	C4-N3	2.07	1.42	1.38
3	A	751	FMN	C8M-C8	2.06	1.54	1.51
4	A	752	NAP	C5A-C4A	-2.06	1.35	1.39
3	A	751	FMN	P-O2P	-2.04	1.47	1.54
4	A	752	NAP	PN-O2N	-2.04	1.45	1.55
2	B	850	FAD	C6A-N1A	2.02	1.41	1.35

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	851	FMN	C9A-C5A-N5	4.39	127.11	122.45
2	A	750	FAD	C4'-C3'-C2'	4.38	120.85	113.57
2	B	850	FAD	C5X-C9A-N10	-3.94	114.41	117.97
3	A	751	FMN	C9A-C5A-N5	3.82	126.51	122.45
3	B	851	FMN	C4'-C3'-C2'	-3.80	107.25	113.57
4	B	852	NAP	N6A-C6A-N1A	3.70	126.61	118.38
4	A	752	NAP	O4B-C1B-N9A	3.68	115.16	108.09
2	B	850	FAD	C4'-C3'-C2'	3.58	119.53	113.57
4	A	752	NAP	N6A-C6A-N1A	3.52	126.22	118.38
3	B	851	FMN	O3P-P-O5'	-3.49	97.57	106.67
4	B	852	NAP	O4B-C1B-N9A	3.41	114.63	108.09
4	A	752	NAP	N3A-C2A-N1A	-3.36	123.49	128.58
2	B	850	FAD	C9A-C5X-N5	3.34	126.00	122.45
4	B	852	NAP	N3A-C2A-N1A	-3.27	123.63	128.58
3	A	751	FMN	O4-C4-N3	-3.27	113.97	120.11
2	B	850	FAD	C9-C9A-N10	3.26	126.23	121.85
2	A	750	FAD	O2-C2-N3	3.23	124.79	118.58
4	B	852	NAP	O7N-C7N-N7N	-3.21	117.98	122.62
2	B	850	FAD	C2'-C1'-N10	-3.20	95.06	110.20
2	B	850	FAD	O5'-C5'-C4'	3.20	117.90	109.36
4	B	852	NAP	C4D-O4D-C1D	3.20	112.85	109.92
3	B	851	FMN	O4-C4-N3	-3.17	114.16	120.11
2	B	850	FAD	O2-C2-N3	3.14	124.61	118.58
4	A	752	NAP	C4D-O4D-C1D	3.09	112.76	109.92
3	A	751	FMN	C4'-C3'-C2'	-3.07	108.47	113.57
3	B	851	FMN	C5A-C9A-N10	-3.00	115.25	117.97
2	A	750	FAD	C9A-C5X-N5	2.99	125.62	122.45
2	A	750	FAD	C5X-C9A-N10	-2.98	115.27	117.97
4	B	852	NAP	O7N-C7N-C3N	2.97	123.23	119.60
3	B	851	FMN	C9-C9A-N10	2.96	125.83	121.85
4	B	852	NAP	C2A-N1A-C6A	2.86	123.42	118.73
3	B	851	FMN	O4'-C4'-C3'	-2.76	102.78	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	752	NAP	C2A-N1A-C6A	2.73	123.22	118.73
4	A	752	NAP	C3B-C2B-C1B	-2.72	97.60	102.81
2	B	850	FAD	C10-N1-C2	2.69	122.68	116.85
3	A	751	FMN	O3P-P-O5'	-2.65	99.75	106.67
2	A	750	FAD	O3'-C3'-C4'	-2.64	102.94	108.93
4	A	752	NAP	O7N-C7N-N7N	-2.57	118.90	122.62
2	A	750	FAD	C10-N1-C2	2.55	122.38	116.85
2	A	750	FAD	C9-C9A-N10	2.52	125.25	121.85
2	A	750	FAD	O5'-C5'-C4'	2.51	116.07	109.36
3	A	751	FMN	C5A-C9A-N10	-2.51	115.70	117.97
3	A	751	FMN	O4'-C4'-C3'	-2.49	103.43	109.25
4	A	752	NAP	O7N-C7N-C3N	2.45	122.59	119.60
2	A	750	FAD	C1B-N9A-C8A	2.45	132.53	127.09
3	A	751	FMN	C9-C9A-N10	2.41	125.10	121.85
4	A	752	NAP	C2B-C1B-N9A	2.35	117.61	113.75
3	B	851	FMN	C7M-C7-C6	-2.35	115.44	119.57
4	A	752	NAP	C5A-C6A-N6A	-2.32	117.53	123.29
4	B	852	NAP	C2N-N1N-C1D	-2.32	114.02	119.13
3	B	851	FMN	C6-C5A-N5	-2.31	114.61	118.44
4	A	752	NAP	C5A-C4A-N3A	-2.31	123.54	126.72
2	A	750	FAD	C2'-C1'-N10	-2.29	99.36	110.20
2	A	750	FAD	C1'-N10-C9A	2.27	125.05	120.63
4	B	852	NAP	C5N-C4N-C3N	2.22	122.55	120.36
4	B	852	NAP	C5A-C6A-N6A	-2.20	117.83	123.29
2	B	850	FAD	O3'-C3'-C4'	-2.20	103.93	108.93
2	B	850	FAD	N3A-C2A-N1A	-2.19	125.27	128.58
4	B	852	NAP	O3X-P2B-O2B	2.17	114.32	105.85
4	B	852	NAP	C5A-C4A-N3A	-2.12	123.80	126.72
4	A	752	NAP	C4A-N9A-C1B	-2.11	121.69	126.63
2	B	850	FAD	C1B-N9A-C8A	2.11	131.78	127.09
2	B	850	FAD	C2B-C1B-N9A	2.11	118.54	113.30
3	B	851	FMN	O5'-P-O1P	2.10	112.12	106.44
3	A	751	FMN	C8M-C8-C7	2.10	125.05	120.76
2	A	750	FAD	C8M-C8-C9	-2.05	115.97	119.57

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	852	NAP	O4D-C1D-N1N-C6N
4	A	752	NAP	O4D-C4D-C5D-O5D
4	B	852	NAP	C2B-C1B-N9A-C8A

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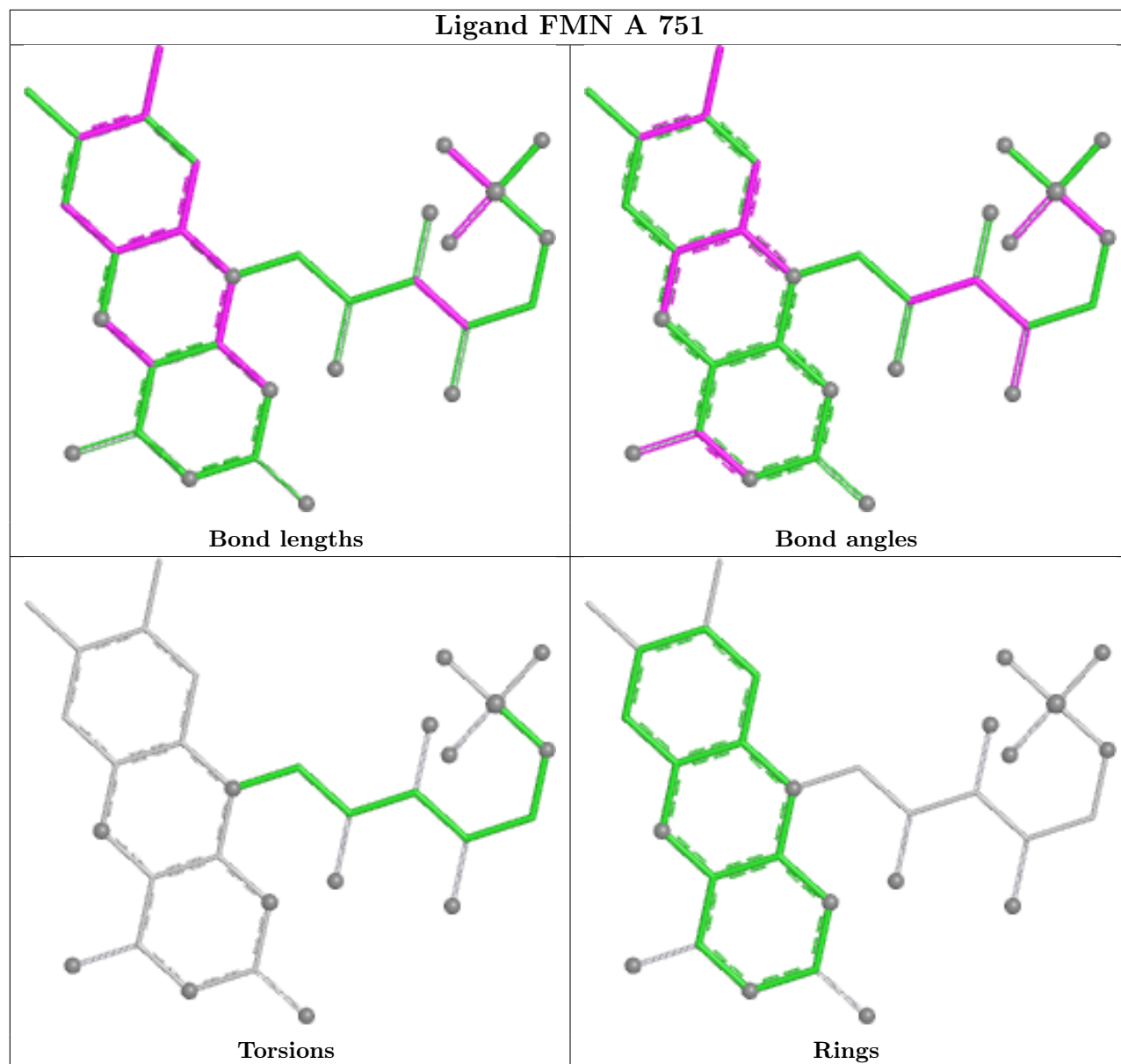
Mol	Chain	Res	Type	Atoms
4	B	852	NAP	O4D-C4D-C5D-O5D
4	A	752	NAP	C3D-C4D-C5D-O5D
2	A	750	FAD	C3'-C4'-C5'-O5'
4	B	852	NAP	C2B-C1B-N9A-C4A
4	A	752	NAP	C2B-C1B-N9A-C8A
2	B	850	FAD	C3'-C4'-C5'-O5'
2	B	850	FAD	PA-O3P-P-O1P
4	A	752	NAP	PA-O3-PN-O1N
4	B	852	NAP	PA-O3-PN-O1N
2	A	750	FAD	PA-O3P-P-O1P
4	A	752	NAP	C2B-C1B-N9A-C4A
4	B	852	NAP	O4D-C1D-N1N-C2N
2	A	750	FAD	PA-O3P-P-O2P
4	B	852	NAP	C2B-O2B-P2B-O2X
4	B	852	NAP	PA-O3-PN-O2N
4	B	852	NAP	C3D-C4D-C5D-O5D

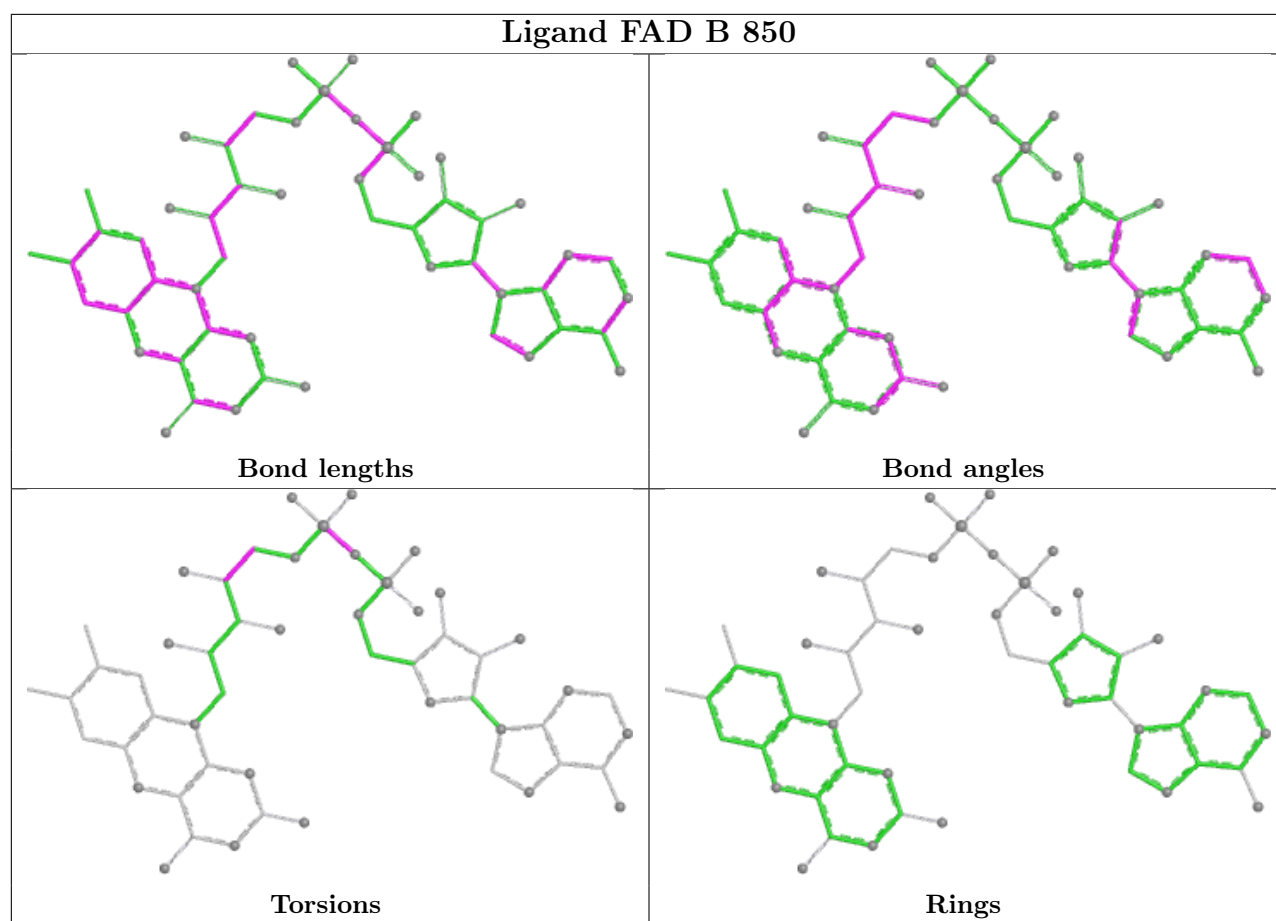
There are no ring outliers.

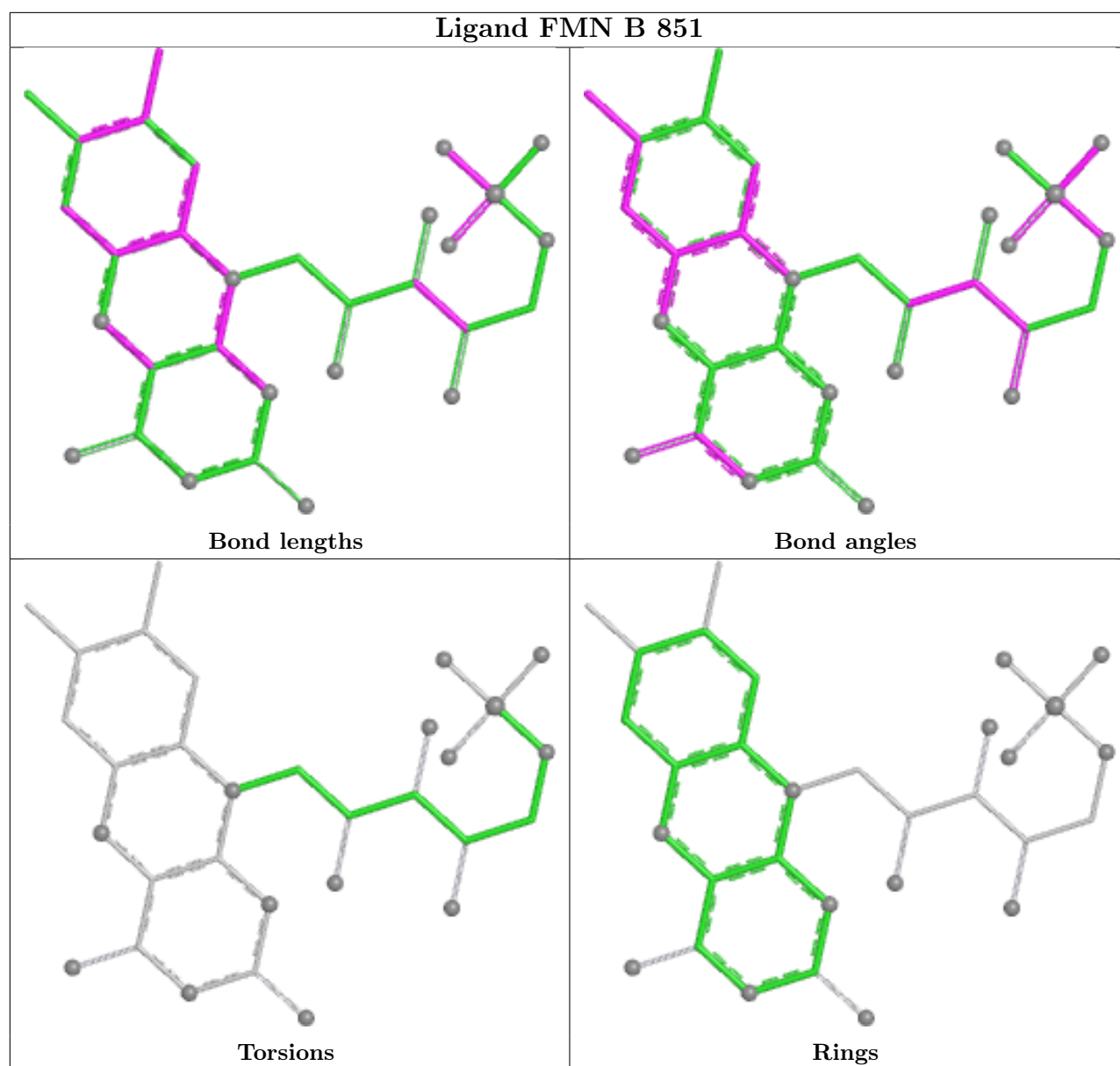
4 monomers are involved in 9 short contacts:

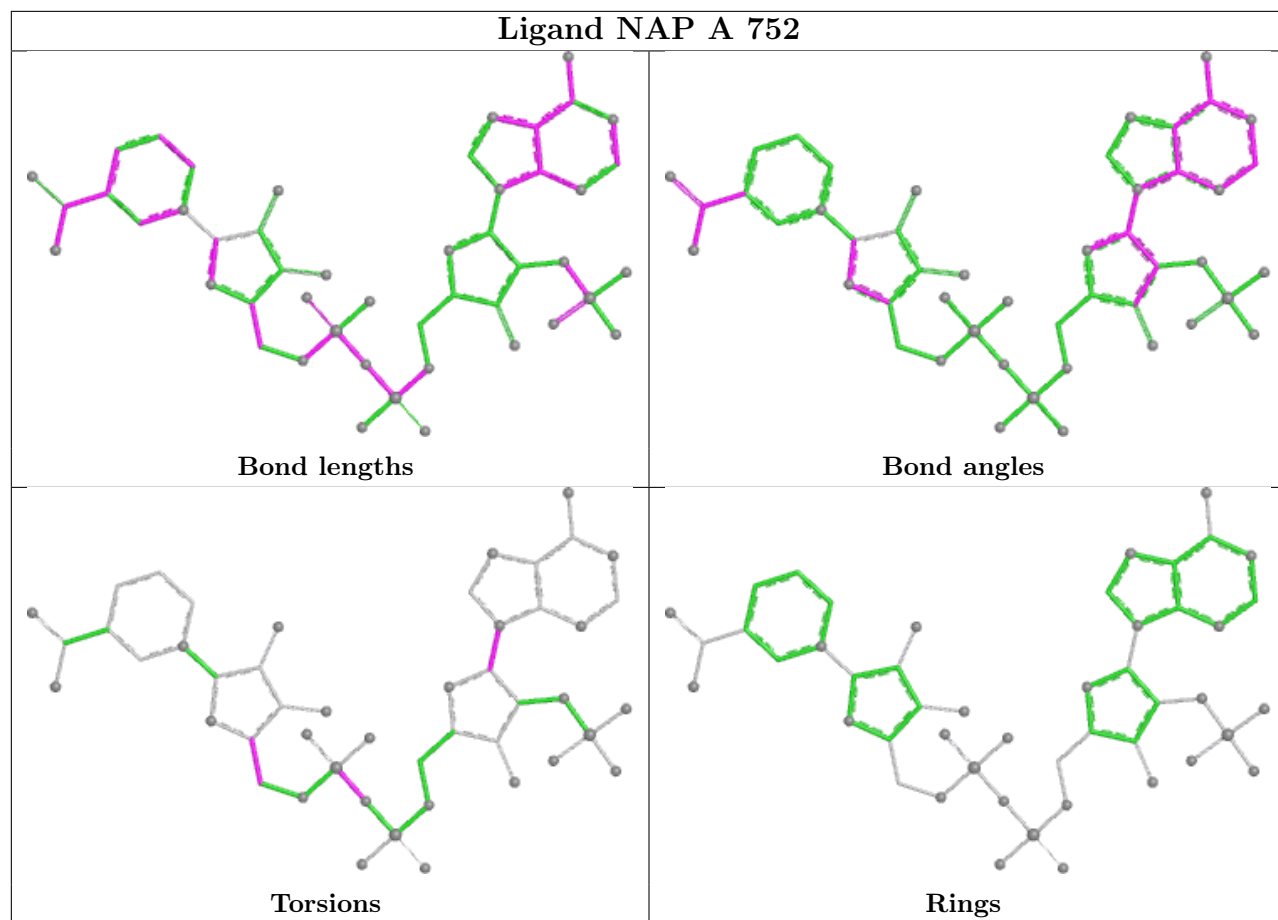
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	751	FMN	4	0
2	B	850	FAD	1	0
3	B	851	FMN	1	0
4	B	852	NAP	3	0

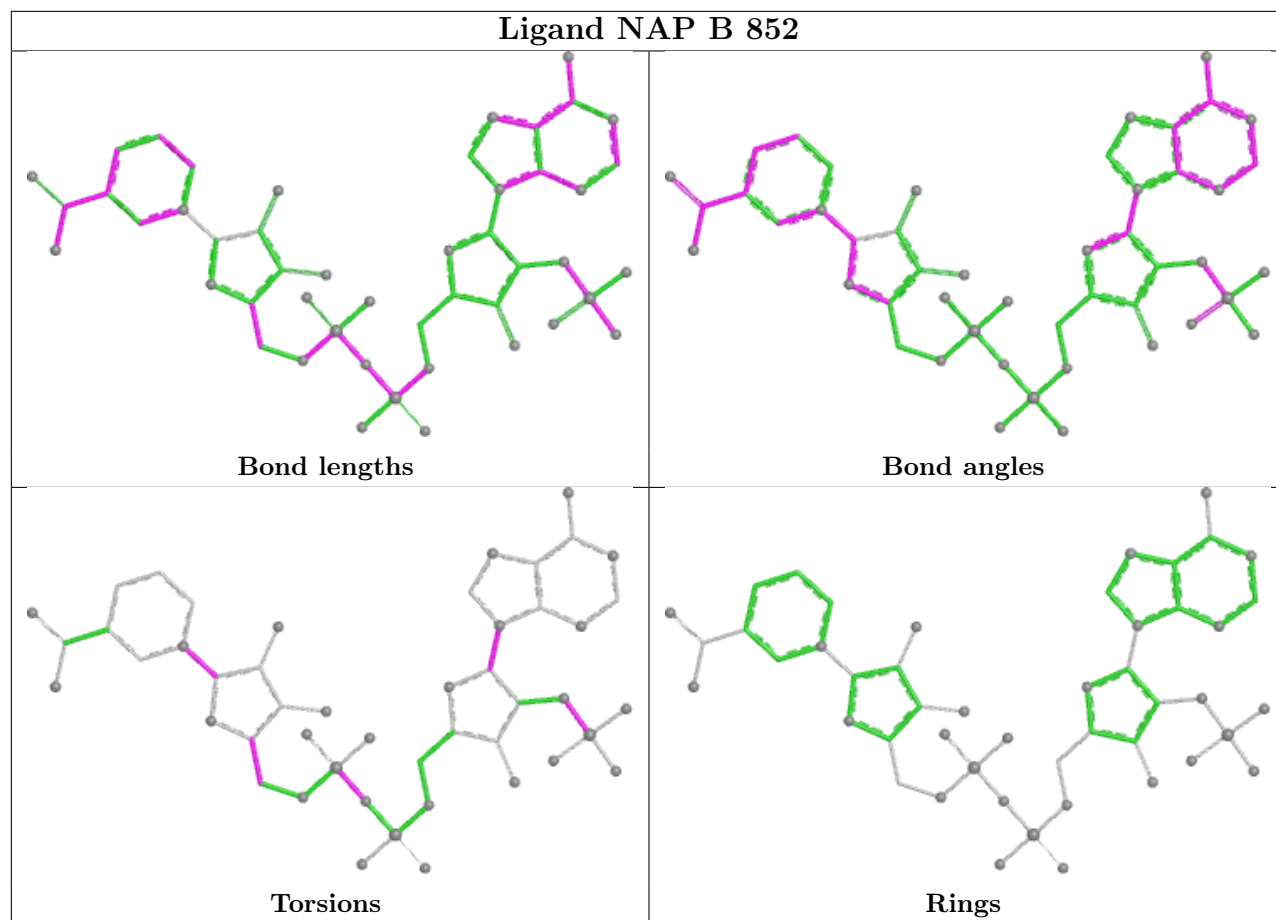
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

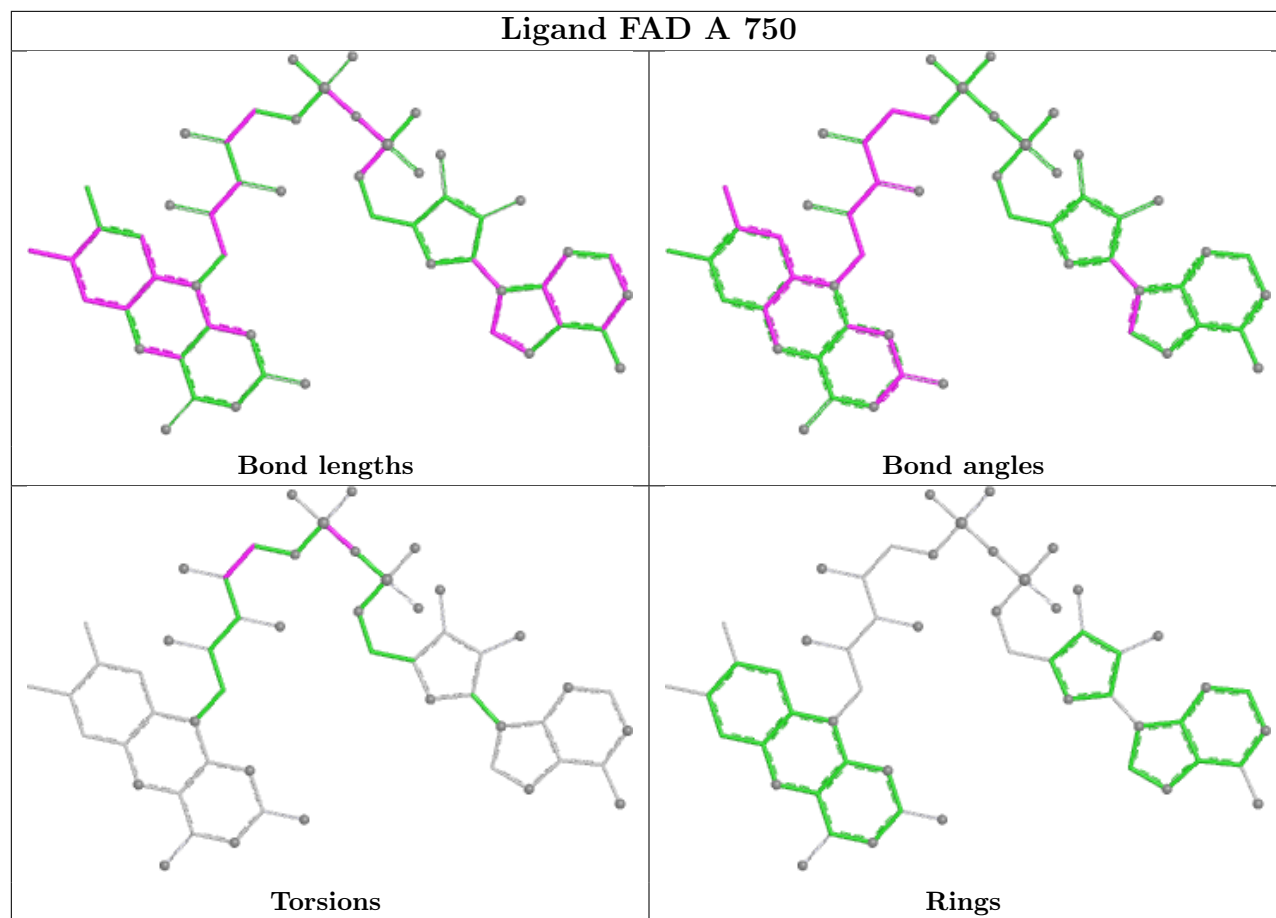












5.7 Other polymers [i](#)

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	613/622 (98%)	-0.66	0	100 100	16, 36, 57, 87	0
1	B	611/622 (98%)	-0.34	2 (0%)	90 89	16, 44, 92, 107	0
All	All	1224/1244 (98%)	-0.50	2 (0%)	91 90	16, 38, 85, 107	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	VAL	2.3
1	B	161	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
3	FMN	B	851	31/31	0.90	0.10	75,91,94,94	0
3	FMN	A	751	31/31	0.95	0.07	37,55,58,58	0
4	NAP	A	752	48/48	0.96	0.08	26,40,70,74	0

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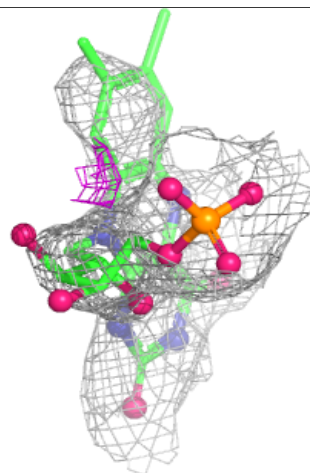
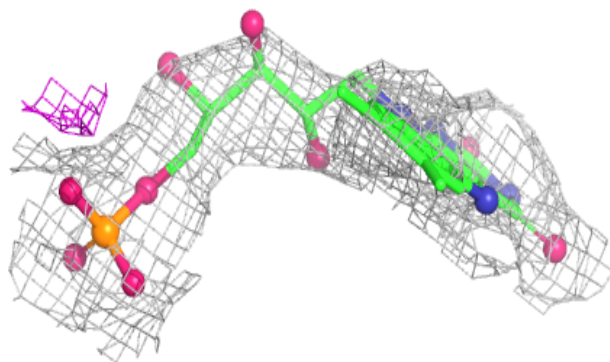
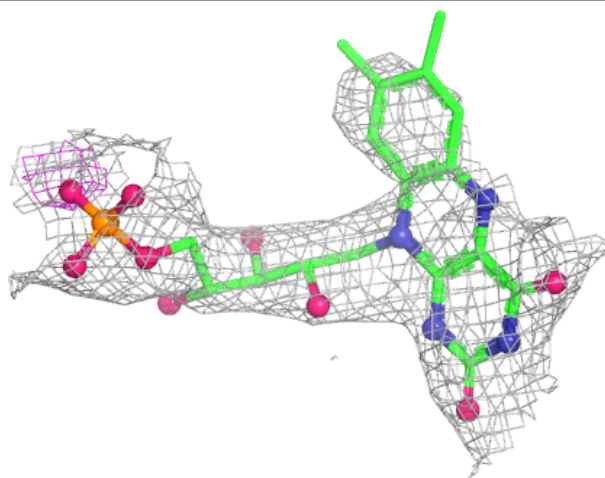
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAP	B	852	48/48	0.96	0.08	26,34,72,74	0
2	FAD	A	750	53/53	0.97	0.06	24,30,35,35	0
2	FAD	B	850	53/53	0.97	0.07	16,21,24,27	0

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.

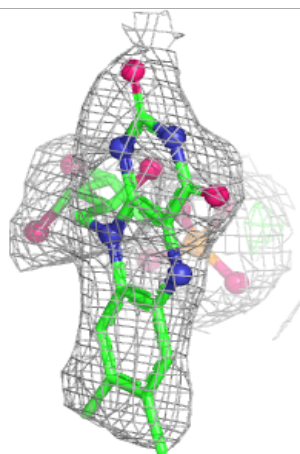
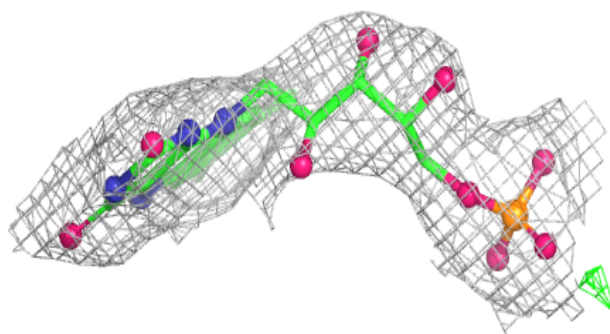
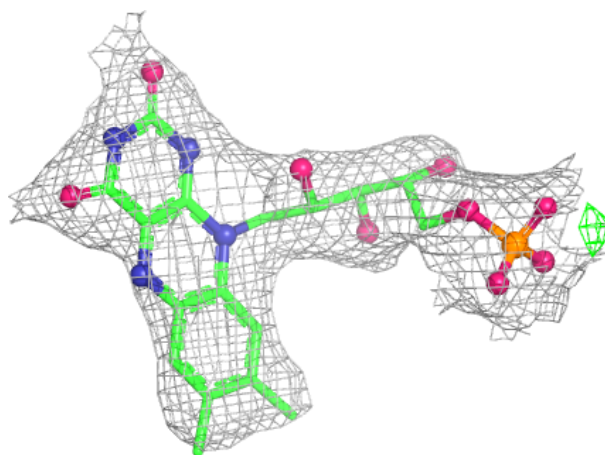
Electron density around FMN B 851:

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



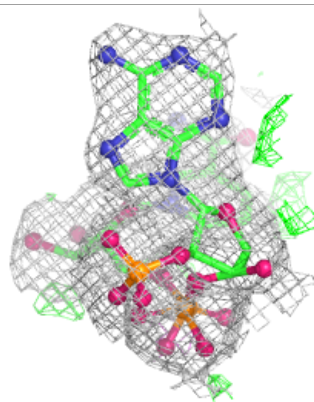
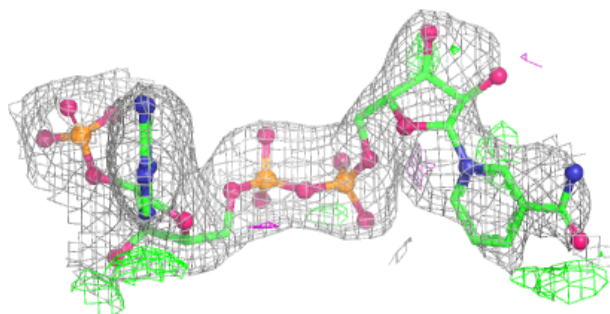
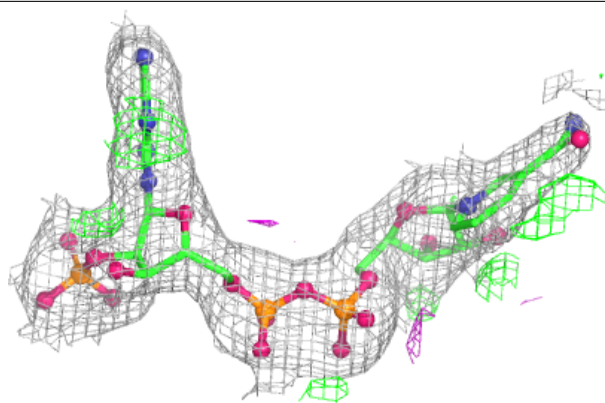
Electron density around FMN A 751:

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

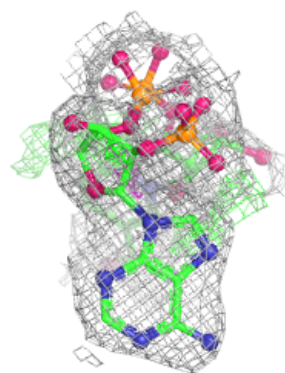
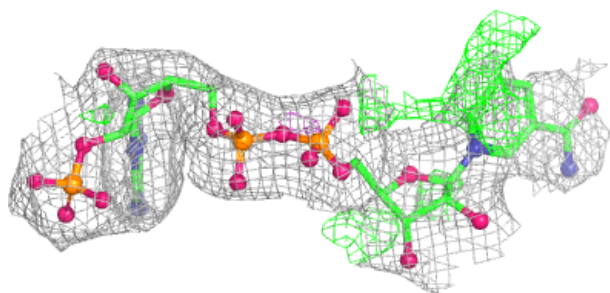
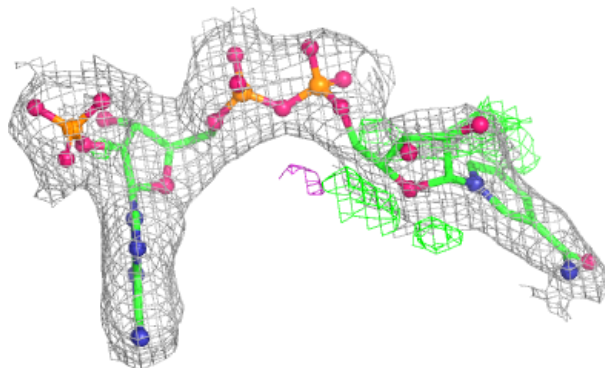


Electron density around NAP A 752:

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

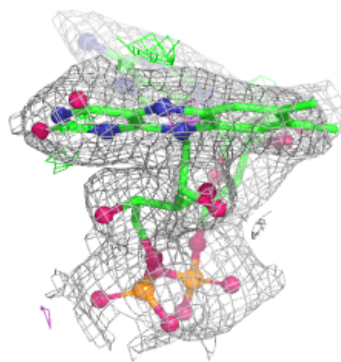
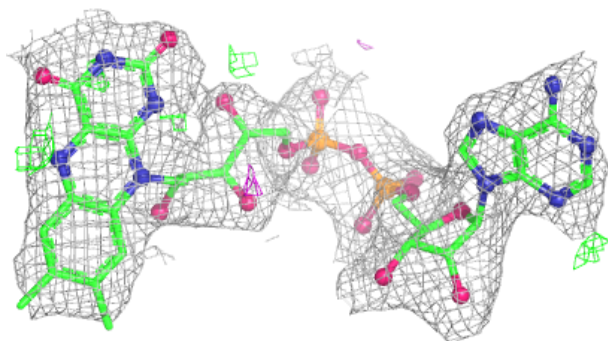
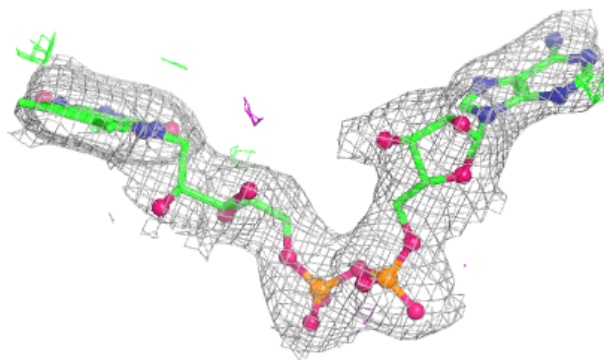
**Electron density around NAP B 852:**

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

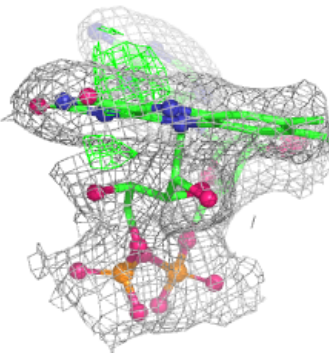
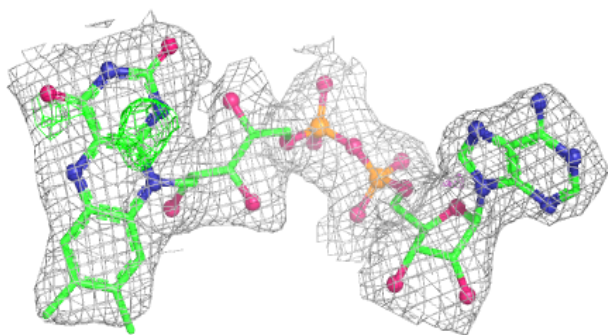
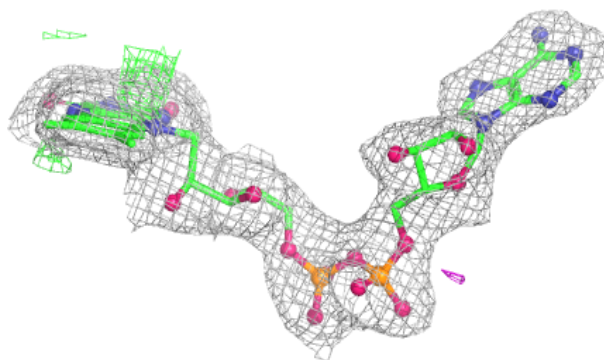


Electron density around FAD A 750:

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

**Electron density around FAD B 850:**

$2mF_o-DF_c$ (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.