



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:36 PM UTC

PDB ID : 6NJR / pdb_00006njr
Title : Spin-Labeled T177C/A637C Mutant of Rat CYPOR
Authors : Xia, C.; Kim, J.J.K.
Deposited on : 2019-01-04
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

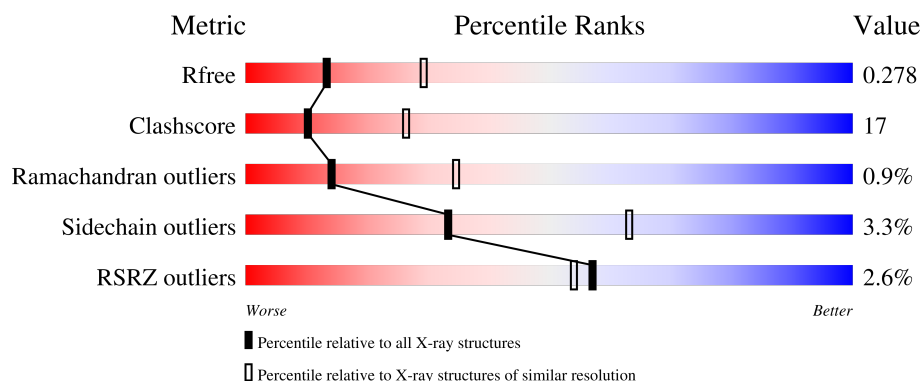
1 Overall quality at a glance

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	% 64% 32% ..
1	B	622	4% 60% 35% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10069 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

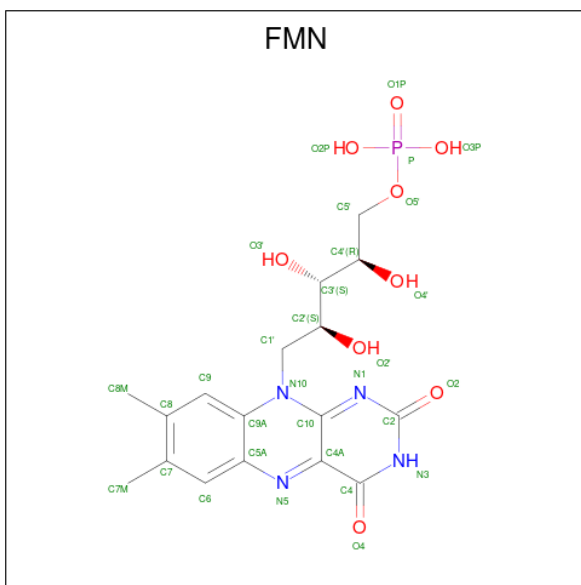
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4888	3105	840	923	20			
1	B	605	Total	C	N	O	S	0	0	0
			4810	3056	825	909	20			

There are 18 discrepancies between the modelled and reference sequences:

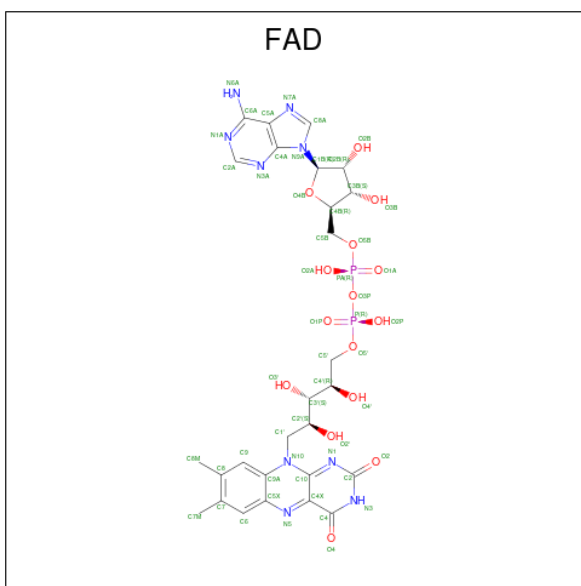
Chain	Residue	Modelled	Actual	Comment	Reference
A	136	ALA	CYS	engineered mutation	UNP P00388
A	177	R1A	THR	engineered mutation	UNP P00388
A	228	ALA	CYS	engineered mutation	UNP P00388
A	363	THR	CYS	engineered mutation	UNP P00388
A	445	LEU	CYS	engineered mutation	UNP P00388
A	472	THR	CYS	engineered mutation	UNP P00388
A	566	ALA	CYS	engineered mutation	UNP P00388
A	630	ALA	CYS	engineered mutation	UNP P00388
A	637	R1A	ALA	engineered mutation	UNP P00388
B	136	ALA	CYS	engineered mutation	UNP P00388
B	177	R1A	THR	engineered mutation	UNP P00388
B	228	ALA	CYS	engineered mutation	UNP P00388
B	363	THR	CYS	engineered mutation	UNP P00388
B	445	LEU	CYS	engineered mutation	UNP P00388
B	472	THR	CYS	engineered mutation	UNP P00388
B	566	ALA	CYS	engineered mutation	UNP P00388
B	630	ALA	CYS	engineered mutation	UNP P00388
B	637	R1A	ALA	engineered mutation	UNP P00388

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



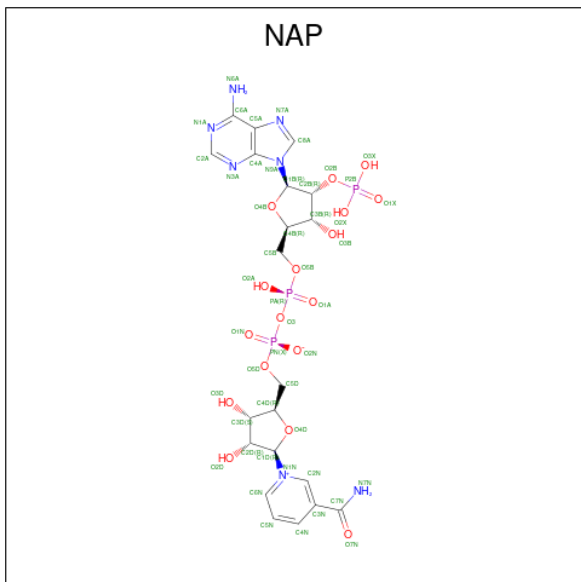
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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 48	C 21	N 7	O 17	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

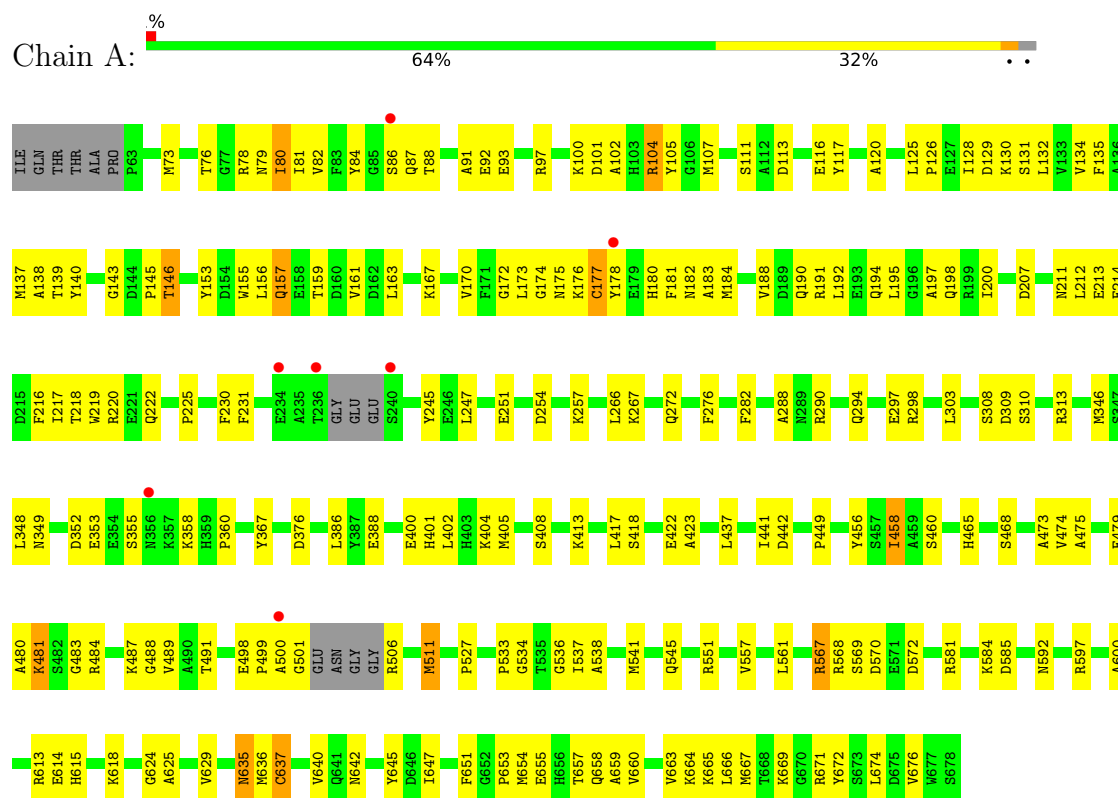
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	55	Total O 55 55	0	0
5	B	52	Total O 52 52	0	0

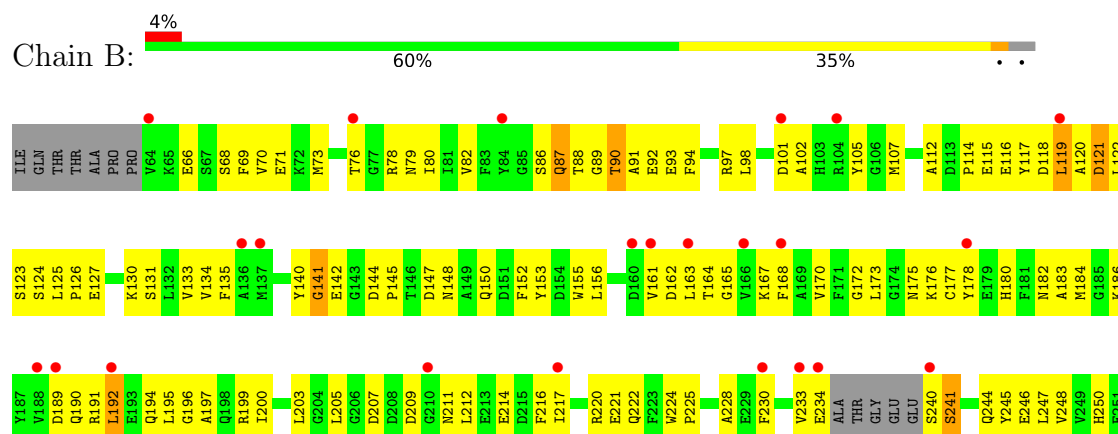
3 Residue-property plots

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



C637	P396	GLY	P396	D252
V640	S397	R506	E398	M253
Q641				V258
N642	H403	S524		K267
Y645	K404	T525		
D646	M405	T526		F276
	A406	P527		D277
	S407			
G652	S408	V531		F282
P653	S409			
V663		G536		N293
K664	G412			
	K413	P539		R298
M667	F540	F540		H299
T668	F543		L417	L300
		S418		R301
R671	W419	V420		
Y672	V421			I307
S673	E422			
L674	A423			S310
D675	R424			K311
V676	R425			
W677	H426			L330
S678	I427			
		S436		I337
				L338
		P439		M346
	D442			L351
	L445			E354
	P449			K357
				K358
	R454			H359
Q590	Y455			P360
	Y456			F361
F595				P362
	V474			T363
Q599	A475			P364
A600				T365
H601				
	E479			D376
Y604	A480			I377
V605	K481			T378
Q606				N379
H607	K487			
				R382
L619	A490			T383
T620	T491			N384
H621	S492			V385
A625	R495			L389
H626				A390
				Q391
V629	A500			E395
	GLY			
	GLU			
M636	ASN			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.27Å 116.01Å 118.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.37 – 2.70 32.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (32.37-2.70) 98.9 (32.37-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.68Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.216 , 0.278 0.216 , 0.278	Depositor DCC
R_{free} test set	1930 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10069	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.99% 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: R1A, 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	0.74	0/4966	1.08	13/6719 (0.2%)
1	B	0.70	0/4886	1.09	15/6616 (0.2%)
All	All	0.72	0/9852	1.08	28/13335 (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	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	GLN	N-CA-C	9.47	121.68	111.36
1	A	251	GLU	N-CA-C	7.57	122.95	112.04
1	A	140	TYR	CB-CA-C	7.41	127.78	112.44
1	A	489	VAL	N-CA-C	7.38	117.91	110.23
1	B	89	GLY	N-CA-C	7.15	125.18	115.32
1	B	230	PHE	N-CA-C	7.03	119.02	111.36
1	B	421	VAL	N-CA-C	6.57	116.72	110.42
1	B	417	LEU	N-CA-C	6.53	120.34	112.38
1	A	635	ASN	CB-CA-C	-6.35	100.97	109.16
1	B	524	SER	N-CA-C	6.15	120.04	112.54
1	A	659	ALA	N-CA-C	-6.10	104.71	111.36
1	B	553	GLN	N-CA-C	-6.09	103.57	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	607	HIS	N-CA-C	-6.03	104.82	111.82
1	B	258	VAL	N-CA-C	5.88	116.78	108.36
1	B	621	HIS	N-CA-C	5.88	117.50	111.14
1	B	427	ILE	N-CA-C	5.82	116.56	110.62
1	A	473	ALA	N-CA-C	5.59	117.89	109.23
1	B	301	MET	N-CA-C	5.58	118.16	109.52
1	A	290	ARG	N-CA-C	5.55	117.71	108.99
1	A	146	THR	N-CA-C	-5.46	103.18	110.55
1	B	87	GLN	CB-CA-C	5.35	118.64	109.65
1	A	218	THR	N-CA-C	-5.27	105.43	111.07
1	B	253	MET	N-CA-C	5.13	118.10	110.14
1	A	481	LYS	N-CA-C	-5.11	106.31	112.54
1	A	117	TYR	N-CA-C	5.10	116.42	109.18
1	A	597	ARG	N-CA-C	5.09	119.22	112.30
1	A	647	ILE	N-CA-C	-5.06	105.39	110.30
1	B	277	ASP	N-CA-C	5.06	114.91	108.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	TYR	Sidechain
1	B	456	TYR	Sidechain
1	B	604	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4888	0	4731	159	0
1	B	4810	0	4596	173	0
2	A	31	0	19	1	0
2	B	31	0	19	3	0
3	A	53	0	31	1	0
3	B	53	0	31	5	0
4	A	48	0	25	5	0
4	B	48	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	55	0	0	4	0
5	B	52	0	0	2	0
All	All	10069	0	9477	333	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 17.

All (333) 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:637:R1A:H71	1:A:676:VAL:CG2	1.72	1.18
1:A:637:R1A:H71	1:A:676:VAL:HG21	1.30	1.11
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.20	1.10
1:B:180:HIS:HB3	1:B:183:ALA:HB2	1.37	1.03
1:B:79:ASN:HB2	1:B:130:LYS:O	1.58	1.03
1:B:168:PHE:CZ	1:B:192:LEU:HB3	1.97	1.00
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.48	0.95
1:B:90:THR:HG23	1:B:382:ARG:NH2	1.83	0.93
1:B:119:LEU:HG	1:B:152:PHE:CD1	2.06	0.91
1:A:637:R1A:C7	1:A:676:VAL:CG2	2.50	0.89
1:A:637:R1A:H71	1:A:676:VAL:HG23	1.54	0.89
1:B:168:PHE:CE1	1:B:192:LEU:HB3	2.10	0.84
1:B:168:PHE:CZ	1:B:192:LEU:CB	2.60	0.84
1:B:454:ARG:HG3	1:B:490:ALA:HB2	1.62	0.81
1:B:175:ASN:HB3	1:B:178:TYR:HD2	1.47	0.80
3:B:702:FAD:H3B	4:B:703:NAP:H4N	1.64	0.79
1:B:186:LYS:HG2	1:B:203:LEU:HD21	1.67	0.76
1:A:665:LYS:O	1:A:669:LYS:HG2	1.86	0.76
1:B:90:THR:HG23	1:B:382:ARG:HH22	1.47	0.75
1:B:70:VAL:HA	1:B:73:MET:HE3	1.68	0.75
1:B:301:MET:HE1	1:B:495:ARG:HA	1.68	0.75
1:A:86:SER:CB	1:A:91:ALA:HB3	2.11	0.74
1:A:637:R1A:C7	1:A:676:VAL:HG21	2.13	0.74
1:A:637:R1A:C7	1:A:676:VAL:HG23	2.18	0.72
1:A:180:HIS:HB3	1:A:183:ALA:HB2	1.71	0.71
1:A:79:ASN:HD21	1:A:107:MET:HB3	1.56	0.70
1:A:533:PRO:HG3	1:A:636:MET:HG3	1.74	0.70
1:B:120:ALA:HA	1:B:155:TRP:CZ2	2.27	0.70
1:A:418:SER:HA	1:A:422:GLU:HB2	1.73	0.69
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.74	0.68
1:B:145:PRO:HB3	1:B:184:MET:SD	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:O	1:A:176:LYS:HG3	1.94	0.68
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.75	0.68
1:B:175:ASN:HB3	1:B:178:TYR:CD2	2.29	0.67
1:B:398:GLU:OE2	1:B:436:SER:HB3	1.93	0.67
1:B:114:PRO:O	1:B:119:LEU:HD23	1.94	0.67
1:A:175:ASN:HB3	1:A:178:TYR:CD1	2.30	0.66
1:A:614:GLU:HA	1:A:651:PHE:CE2	2.30	0.66
1:A:86:SER:HB2	1:A:91:ALA:CB	2.12	0.66
1:B:376:ASP:OD2	1:B:379:ASN:HB2	1.95	0.66
1:B:454:ARG:HG3	1:B:490:ALA:CB	2.26	0.66
1:A:76:THR:HB	1:A:78:ARG:HD2	1.77	0.66
1:B:228:ALA:HB1	1:B:233:VAL:O	1.97	0.65
1:B:119:LEU:O	1:B:122:LEU:HG	1.97	0.65
1:A:219:TRP:HB2	5:A:806:HOH:O	1.96	0.65
1:B:454:ARG:HD2	3:B:702:FAD:O2P	1.97	0.65
1:B:637:R1A:SD	1:B:676:VAL:HG21	2.37	0.65
1:A:276:PHE:CG	1:A:282:PHE:HB2	2.32	0.65
1:B:115:GLU:HB2	1:B:148:ASN:O	1.97	0.65
1:B:70:VAL:HG11	1:B:124:SER:O	1.96	0.64
1:A:423:ALA:O	1:A:480:ALA:HB1	1.98	0.64
1:B:194:GLN:O	1:B:195:LEU:HD12	1.98	0.64
1:A:214:GLU:HG2	1:A:417:LEU:HD21	1.79	0.64
1:B:250:HIS:CG	1:B:253:MET:HE3	2.33	0.64
1:A:97:ARG:HA	1:A:100:LYS:HE3	1.80	0.63
1:B:90:THR:CG2	1:B:382:ARG:HH22	2.10	0.63
1:B:228:ALA:CB	1:B:233:VAL:O	2.45	0.63
1:B:191:ARG:O	1:B:191:ARG:HD3	1.98	0.63
1:B:282:PHE:HE2	1:B:307:ILE:HA	1.64	0.63
1:B:120:ALA:C	1:B:122:LEU:H	2.07	0.63
1:A:418:SER:O	1:A:422:GLU:HB3	1.99	0.63
1:A:418:SER:HA	1:A:422:GLU:CB	2.30	0.62
1:A:458:ILE:HG22	1:A:460:SER:H	1.64	0.62
1:A:475:ALA:HA	1:A:491:THR:HB	1.81	0.62
1:B:300:LEU:HD13	1:B:574:LEU:HD21	1.82	0.62
1:B:180:HIS:HB3	1:B:183:ALA:CB	2.22	0.61
1:B:97:ARG:CZ	1:B:384:ASN:HB3	2.31	0.61
1:A:178:TYR:CD2	1:A:637:R1A:O1	2.54	0.61
1:B:86:SER:CB	1:B:91:ALA:HB3	2.28	0.60
1:B:69:PHE:HZ	1:B:122:LEU:HD23	1.66	0.60
1:B:125:LEU:N	1:B:126:PRO:HD2	2.16	0.60
1:A:176:LYS:C	1:A:178:TYR:H	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:703:NAP:O2N	4:A:703:NAP:H4D	2.01	0.60
1:A:139:THR:CG2	1:A:143:GLY:HA2	2.31	0.60
1:A:481:LYS:HE2	1:B:481:LYS:HE3	1.84	0.60
1:B:330:LEU:HD22	1:B:377:ILE:HD12	1.84	0.60
1:B:186:LYS:HG2	1:B:203:LEU:CD2	2.32	0.59
1:B:175:ASN:OD1	1:B:209:ASP:HB2	2.02	0.59
1:B:409:SER:HA	1:B:413:LYS:HB2	1.83	0.59
1:B:147:ASP:HA	1:B:150:GLN:HG2	1.84	0.59
1:A:551:ARG:HG2	1:A:557:VAL:CG2	2.32	0.58
1:B:91:ALA:HB2	1:B:173:LEU:HD22	1.86	0.58
1:B:536:GLY:O	1:B:539:PRO:HD2	2.04	0.58
1:B:168:PHE:CZ	1:B:192:LEU:HB2	2.39	0.58
1:B:540:PHE:HA	1:B:543:PHE:HB2	1.85	0.58
1:B:664:LYS:O	1:B:668:THR:HG23	2.04	0.57
1:B:126:PRO:HB3	1:B:165:GLY:O	2.04	0.57
1:B:310:SER:O	1:B:311:LYS:HB2	2.04	0.57
1:B:135:PHE:HB2	1:B:170:VAL:HG22	1.85	0.57
1:A:176:LYS:HA	1:A:181:PHE:CD1	2.40	0.57
1:A:167:LYS:HE3	1:A:198:GLN:OE1	2.04	0.57
1:B:114:PRO:O	1:B:119:LEU:CD2	2.53	0.57
1:B:293:ASN:ND2	1:B:298:ARG:O	2.38	0.57
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.85	0.56
1:A:551:ARG:HG2	1:A:557:VAL:HG21	1.87	0.56
1:A:355:SER:O	1:A:358:LYS:NZ	2.38	0.56
1:B:363:THR:HB	1:B:364:PRO:HA	1.87	0.56
1:A:222:GLN:O	1:A:225:PRO:HD2	2.05	0.56
1:A:655:GLU:HB2	1:A:658:GLN:OE1	2.06	0.56
1:A:665:LYS:HZ1	1:A:669:LYS:HE3	1.70	0.56
1:B:276:PHE:CG	1:B:282:PHE:HB2	2.41	0.55
1:B:162:ASP:C	1:B:164:THR:H	2.15	0.55
1:B:293:ASN:HB3	1:B:300:LEU:HD12	1.88	0.55
1:A:672:TYR:HE1	1:A:674:LEU:HD21	1.72	0.54
1:B:221:GLU:CD	1:B:408:SER:HB3	2.32	0.54
1:A:163:LEU:HD12	1:A:195:LEU:HB2	1.89	0.54
1:A:636:MET:HA	4:A:703:NAP:N1A	2.23	0.54
1:A:637:R1A:O	1:A:640:VAL:N	2.41	0.54
1:B:167:LYS:CB	1:B:200:ILE:HD11	2.37	0.54
1:A:625:ALA:N	1:A:671:ARG:HH21	2.05	0.54
1:A:135:PHE:HB2	1:A:170:VAL:HG22	1.90	0.54
1:A:73:MET:HE3	1:A:81:ILE:HB	1.89	0.53
1:A:214:GLU:CG	1:A:417:LEU:HD21	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:VAL:CG1	1:A:664:LYS:HE2	2.37	0.53
1:A:167:LYS:HE2	1:A:230:PHE:CZ	2.43	0.53
1:B:299:HIS:NE2	1:B:301:MET:HE3	2.23	0.53
1:B:168:PHE:CE2	1:B:192:LEU:HB2	2.44	0.53
1:A:498:GLU:C	1:A:500:ALA:H	2.17	0.53
1:A:498:GLU:O	1:A:500:ALA:N	2.42	0.52
1:B:423:ALA:HA	1:B:481:LYS:HB2	1.91	0.52
1:A:460:SER:HA	1:A:545:GLN:OE1	2.09	0.52
1:B:361:PHE:O	1:B:363:THR:HG23	2.09	0.52
1:B:168:PHE:HD1	1:B:197:ALA:HB1	1.74	0.52
1:A:474:VAL:HG11	4:A:703:NAP:H52N	1.92	0.52
1:A:87:GLN:O	1:A:87:GLN:HG2	2.09	0.52
1:B:101:ASP:HB3	1:B:224:TRP:CE2	2.44	0.52
1:A:79:ASN:ND2	1:A:80:ILE:HG22	2.25	0.52
1:B:120:ALA:O	1:B:122:LEU:N	2.42	0.52
1:B:599:GLN:HG3	1:B:601:HIS:CE1	2.45	0.52
1:B:90:THR:CG2	1:B:382:ARG:NH2	2.63	0.51
1:B:566:ALA:O	1:B:595:PHE:HA	2.10	0.51
1:B:189:ASP:HB2	1:B:203:LEU:HD13	1.92	0.51
1:B:97:ARG:NE	1:B:384:ASN:HB3	2.25	0.51
1:B:118:ASP:O	1:B:121:ASP:OD1	2.29	0.51
1:B:475:ALA:HA	1:B:491:THR:HB	1.91	0.51
1:B:79:ASN:O	1:B:131:SER:HA	2.11	0.51
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.93	0.51
1:B:69:PHE:CZ	1:B:122:LEU:HD23	2.46	0.51
1:B:168:PHE:CD1	1:B:197:ALA:HB1	2.45	0.50
1:B:246:GLU:HG3	1:B:351:LEU:CD2	2.41	0.50
1:B:87:GLN:HB3	1:B:140:TYR:CZ	2.47	0.50
1:B:115:GLU:C	1:B:117:TYR:H	2.18	0.50
1:B:240:SER:O	1:B:241:SER:CB	2.58	0.50
1:A:665:LYS:NZ	1:A:669:LYS:HE3	2.25	0.50
1:A:132:LEU:HD11	1:A:200:ILE:HG21	1.93	0.50
1:B:168:PHE:CE2	1:B:192:LEU:CB	2.95	0.50
1:B:245:TYR:CE2	1:B:360:PRO:HD3	2.46	0.50
1:A:349:ASN:HA	1:A:358:LYS:O	2.11	0.50
1:B:559:GLU:OE2	1:B:619:LEU:HD21	2.12	0.50
1:B:216:PHE:O	1:B:220:ARG:HB3	2.12	0.50
1:A:272:GLN:HG3	5:A:849:HOH:O	2.11	0.49
1:A:657:THR:HG22	1:A:658:GLN:HE21	1.76	0.49
1:B:123:SER:O	1:B:126:PRO:HD2	2.12	0.49
1:B:395:GLU:OE1	1:B:396:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PHE:O	1:A:220:ARG:HB2	2.12	0.49
1:B:548:ALA:O	1:B:552:GLU:HG2	2.13	0.49
1:A:211:ASN:OD1	1:A:213:GLU:HB3	2.12	0.49
1:A:498:GLU:C	1:A:500:ALA:N	2.70	0.49
1:A:581:ARG:HH12	1:A:584:LYS:HG2	1.78	0.49
1:A:178:TYR:CD2	2:A:701:FMN:C4A	2.96	0.48
1:A:247:LEU:HA	1:A:348:LEU:HD23	1.95	0.48
1:A:113:ASP:HB3	1:A:116:GLU:HG3	1.95	0.48
1:A:104:ARG:HB2	1:A:105:TYR:CE1	2.48	0.48
1:A:222:GLN:C	1:A:225:PRO:HD2	2.38	0.48
1:A:159:THR:OG1	1:A:161:VAL:HG12	2.14	0.48
1:A:511:MET:SD	1:A:511:MET:C	2.97	0.48
1:A:645:TYR:CE1	1:A:660:VAL:HA	2.49	0.48
1:B:189:ASP:OD1	1:B:199:ARG:NE	2.37	0.48
1:B:203:LEU:CD2	1:B:205:LEU:HD21	2.44	0.48
1:B:577:GLU:CD	1:B:577:GLU:H	2.22	0.48
1:B:228:ALA:HB1	1:B:234:GLU:HA	1.96	0.47
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.96	0.47
1:A:138:ALA:O	1:A:146:THR:HG23	2.14	0.47
1:A:298:ARG:HD3	5:A:837:HOH:O	2.14	0.47
1:B:301:MET:HE1	1:B:495:ARG:HG3	1.96	0.47
1:A:245:TYR:CE1	1:A:360:PRO:HD3	2.50	0.47
1:B:636:MET:O	1:B:640:VAL:HG23	2.14	0.47
1:A:667:MET:HG2	1:A:672:TYR:HB3	1.96	0.47
1:A:101:ASP:OD1	1:A:220:ARG:NH2	2.48	0.47
1:A:184:MET:HE3	1:A:188:VAL:HG23	1.97	0.47
1:A:615:HIS:O	1:A:618:LYS:HB3	2.15	0.47
1:B:176:LYS:C	1:B:178:TYR:H	2.23	0.47
1:B:301:MET:HE1	1:B:495:ARG:CA	2.40	0.47
1:B:403:HIS:C	1:B:405:MET:H	2.22	0.47
1:B:404:LYS:O	1:B:412:GLY:HA3	2.14	0.47
1:B:178:TYR:CE2	2:B:701:FMN:C10	2.98	0.47
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.97	0.47
1:B:152:PHE:O	1:B:156:LEU:HG	2.15	0.47
1:B:76:THR:OG1	1:B:78:ARG:HG2	2.15	0.47
1:B:125:LEU:N	1:B:126:PRO:CD	2.78	0.47
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.96	0.46
1:B:418:SER:HA	1:B:422:GLU:HB3	1.97	0.46
1:B:247:LEU:HD22	1:B:442:ASP:HB3	1.97	0.46
1:B:673:SER:O	1:B:674:LEU:HD23	2.16	0.46
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:HIS:CE1	5:B:828:HOH:O	2.68	0.46
1:A:297:GLU:C	1:A:298:ARG:HG3	2.40	0.46
1:A:534:GLY:C	1:A:536:GLY:H	2.24	0.46
1:B:419:TRP:O	1:B:425:ARG:HD2	2.14	0.46
1:A:79:ASN:O	1:A:131:SER:HA	2.15	0.46
4:A:703:NAP:O2D	4:A:703:NAP:H2N	2.16	0.46
1:B:385:VAL:O	1:B:389:LEU:HG	2.15	0.46
1:B:636:MET:SD	1:B:636:MET:C	2.99	0.46
1:A:145:PRO:HG2	1:A:153:TYR:CD2	2.51	0.46
1:A:402:LEU:HD11	1:A:437:LEU:HD22	1.97	0.46
1:A:663:VAL:HA	1:A:666:LEU:HD12	1.98	0.46
1:B:180:HIS:CB	1:B:183:ALA:HB2	2.26	0.46
1:A:145:PRO:HG2	1:A:153:TYR:CG	2.51	0.46
1:A:400:GLU:HG3	1:A:404:LYS:HE3	1.97	0.46
1:B:93:GLU:O	1:B:97:ARG:HG3	2.15	0.46
1:A:184:MET:HE3	1:A:188:VAL:CG2	2.46	0.45
1:A:541:MET:O	1:A:545:GLN:HG3	2.15	0.45
1:B:120:ALA:C	1:B:122:LEU:N	2.74	0.45
1:A:441:ILE:HG23	1:A:442:ASP:N	2.29	0.45
1:A:592:ASN:HA	5:A:846:HOH:O	2.16	0.45
1:B:203:LEU:HD21	1:B:205:LEU:HD21	1.97	0.45
1:A:80:ILE:HG13	1:A:81:ILE:N	2.31	0.45
1:A:481:LYS:C	1:A:483:GLY:N	2.72	0.45
1:B:164:THR:HA	1:B:196:GLY:HA3	1.98	0.45
1:A:408:SER:O	1:A:413:LYS:HD2	2.16	0.45
1:A:660:VAL:HG12	1:A:664:LYS:HE2	1.99	0.45
1:B:125:LEU:C	1:B:127:GLU:H	2.23	0.45
1:B:677:TRP:CZ2	3:B:702:FAD:C4	3.00	0.45
1:A:581:ARG:CZ	1:A:585:ASP:OD1	2.65	0.45
1:B:68:SER:HB3	1:B:71:GLU:CD	2.42	0.45
1:B:140:TYR:O	1:B:141:GLY:C	2.60	0.45
1:A:76:THR:HG22	1:A:78:ARG:NH1	2.32	0.45
1:A:500:ALA:O	1:A:501:GLY:C	2.60	0.45
1:A:101:ASP:O	1:A:102:ALA:C	2.60	0.45
1:A:177:R1A:HB2	1:A:177:R1A:HE3	1.24	0.45
1:B:92:GLU:OE1	1:B:357:LYS:NZ	2.50	0.44
3:B:702:FAD:HM71	3:B:702:FAD:HM83	1.74	0.44
1:A:488:GLY:HA2	3:A:702:FAD:O1A	2.18	0.44
1:B:94:PHE:HD2	1:B:173:LEU:HD11	1.81	0.44
1:B:487:LYS:HE2	1:B:492:SER:OG	2.18	0.44
1:A:294:GLN:CD	1:A:294:GLN:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:PHE:CD2	1:B:173:LEU:HD11	2.52	0.44
1:B:98:LEU:O	1:B:101:ASP:HB2	2.17	0.44
1:A:276:PHE:CD1	1:A:282:PHE:HB2	2.53	0.44
1:B:120:ALA:HB2	1:B:155:TRP:NE1	2.32	0.44
1:B:246:GLU:HG3	1:B:351:LEU:HD23	1.98	0.44
1:B:606:GLN:OE1	4:B:703:NAP:H2A	2.18	0.44
1:B:80:ILE:HD12	1:B:102:ALA:HB2	1.99	0.44
1:A:288:ALA:O	1:A:303:LEU:HA	2.17	0.44
1:A:401:HIS:O	1:A:405:MET:HG2	2.18	0.44
1:A:600:ALA:HB1	1:B:337:ILE:HB	2.00	0.44
1:A:78:ARG:HH11	1:A:78:ARG:HG3	1.83	0.43
1:B:147:ASP:O	1:B:150:GLN:HG2	2.17	0.43
1:B:69:PHE:HD2	1:B:73:MET:HE2	1.84	0.43
1:B:120:ALA:HA	1:B:155:TRP:CE2	2.53	0.43
1:A:137:MET:CE	1:A:184:MET:HE2	2.49	0.43
1:A:423:ALA:HA	1:A:481:LYS:HB2	1.99	0.43
1:B:133:VAL:O	1:B:133:VAL:HG13	2.18	0.43
1:A:134:VAL:HG12	1:A:135:PHE:N	2.33	0.43
1:A:613:ARG:HG2	1:A:613:ARG:NH1	2.33	0.43
1:A:282:PHE:CZ	1:A:310:SER:HB3	2.54	0.43
1:B:526:THR:HA	1:B:527:PRO:HD3	1.83	0.43
1:A:93:GLU:OE2	1:A:97:ARG:HD2	2.19	0.42
1:B:217:ILE:CG2	1:B:408:SER:HA	2.49	0.42
1:B:391:GLN:HB3	5:B:847:HOH:O	2.19	0.42
1:A:128:ILE:O	1:A:131:SER:HB3	2.18	0.42
1:A:157:GLN:HE21	1:A:157:GLN:HB2	1.59	0.42
1:B:125:LEU:HG	1:B:131:SER:HB3	2.01	0.42
1:B:176:LYS:HG3	1:B:207:ASP:CG	2.43	0.42
1:A:346:MET:HG2	1:A:367:TYR:CE1	2.54	0.42
1:B:172:GLY:C	1:B:182:ASN:OD1	2.63	0.42
1:B:548:ALA:HB2	1:B:587:ALA:HB1	2.01	0.42
1:B:642:ASN:HA	1:B:645:TYR:CD2	2.55	0.42
1:A:636:MET:HA	4:A:703:NAP:C6A	2.49	0.42
1:A:76:THR:HG22	1:A:76:THR:O	2.20	0.42
1:A:561:LEU:N	1:A:561:LEU:HD12	2.34	0.42
1:A:665:LYS:O	1:A:669:LYS:CG	2.62	0.42
1:A:257:LYS:CA	1:A:266:LEU:HD21	2.47	0.42
1:A:266:LEU:O	1:A:267:LYS:HB2	2.19	0.42
1:B:222:GLN:C	1:B:225:PRO:HD2	2.44	0.42
1:B:244:GLN:O	1:B:244:GLN:HG3	2.20	0.42
1:A:105:TYR:O	1:A:107:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ALA:HA	1:A:155:TRP:CZ2	2.54	0.42
1:A:282:PHE:CE2	1:A:310:SER:HB3	2.54	0.42
1:A:506:ARG:HE	1:A:506:ARG:HB3	1.52	0.42
1:B:112:ALA:HB1	1:B:117:TYR:HE2	1.84	0.42
1:B:409:SER:HA	1:B:413:LYS:CB	2.50	0.42
1:A:272:GLN:OE1	1:A:282:PHE:HA	2.20	0.42
1:A:216:PHE:CE2	1:A:220:ARG:HD2	2.55	0.42
1:A:465:HIS:HB3	1:A:468:SER:HB3	2.02	0.42
1:A:125:LEU:N	1:A:126:PRO:CD	2.83	0.41
1:A:174:GLY:O	1:A:207:ASP:HA	2.20	0.41
1:A:568:ARG:NH2	1:A:570:ASP:OD1	2.53	0.41
1:A:190:GLN:O	1:A:194:GLN:HG3	2.20	0.41
1:A:245:TYR:CD1	1:A:360:PRO:HD3	2.55	0.41
1:B:250:HIS:HB3	1:B:253:MET:HG2	2.01	0.41
1:A:352:ASP:OD1	1:A:355:SER:HB2	2.20	0.41
1:A:624:GLY:HA2	1:A:671:ARG:NH2	2.35	0.41
1:B:73:MET:HB3	1:B:78:ARG:O	2.21	0.41
1:A:172:GLY:C	1:A:182:ASN:OD1	2.64	0.41
1:A:130:LYS:HA	1:A:231:PHE:CE1	2.56	0.41
1:B:76:THR:HG23	1:B:354:GLU:OE2	2.21	0.41
1:B:338:LEU:HD22	1:B:439:PRO:O	2.20	0.41
1:A:481:LYS:C	1:A:483:GLY:H	2.29	0.41
1:B:105:TYR:C	1:B:107:MET:H	2.29	0.41
1:B:214:GLU:OE1	1:B:413:LYS:HG3	2.21	0.41
1:B:383:THR:HB	1:B:406:ALA:HA	2.02	0.41
1:A:84:TYR:CE2	1:A:92:GLU:HG3	2.55	0.41
1:A:192:LEU:O	1:A:197:ALA:HB3	2.21	0.41
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.83	0.41
1:B:247:LEU:HD12	1:B:248:VAL:N	2.36	0.41
1:B:531:VAL:O	1:B:629:VAL:HA	2.21	0.41
1:B:626:HIS:CD2	1:B:671:ARG:HG2	2.55	0.41
1:B:663:VAL:HG12	1:B:667:MET:HE3	2.02	0.41
1:A:82:VAL:O	1:A:111:SER:HA	2.21	0.41
1:A:213:GLU:O	1:A:217:ILE:HG13	2.21	0.41
1:A:308:SER:O	1:A:309:ASP:HB2	2.21	0.41
1:A:417:LEU:O	1:A:422:GLU:HB2	2.21	0.41
1:A:537:ILE:HG23	1:A:538:ALA:N	2.35	0.41
1:B:119:LEU:CG	1:B:152:PHE:CD1	2.91	0.41
1:B:258:VAL:HG13	1:B:365:THR:HA	2.02	0.41
1:B:301:MET:HE1	1:B:495:ARG:CB	2.51	0.41
1:A:91:ALA:HB2	1:A:173:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ASN:HA	1:A:645:TYR:CD2	2.56	0.41
1:B:178:TYR:CZ	2:B:701:FMN:C5A	3.04	0.41
1:B:677:TRP:CZ2	3:B:702:FAD:C4X	3.04	0.40
1:B:134:VAL:HG12	1:B:135:PHE:N	2.36	0.40
1:B:145:PRO:HG3	1:B:153:TYR:CG	2.56	0.40
1:B:652:GLY:N	1:B:653:PRO:HA	2.36	0.40
1:A:479:GLU:OE1	1:B:479:GLU:HG3	2.21	0.40
1:A:567:ARG:HG3	1:A:572:ASP:OD2	2.22	0.40
1:A:572:ASP:OD1	1:A:572:ASP:N	2.54	0.40
1:B:178:TYR:OH	2:B:701:FMN:C5A	2.70	0.40
1:B:245:TYR:CD2	1:B:360:PRO:HD3	2.57	0.40
1:B:406:ALA:O	1:B:407:SER:C	2.63	0.40
1:A:138:ALA:HA	1:A:173:LEU:O	2.21	0.40
1:B:346:MET:HE3	1:B:365:THR:O	2.21	0.40
1:A:653:PRO:O	1:A:654:MET:HB3	2.21	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	601/622 (97%)	554 (92%)	45 (8%)	2 (0%)	36 60
1	B	597/622 (96%)	537 (90%)	51 (8%)	9 (2%)	8 22
All	All	1198/1244 (96%)	1091 (91%)	96 (8%)	11 (1%)	14 35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	SER
1	B	66	GLU
1	B	141	GLY

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Mol	Chain	Res	Type
1	A	104	ARG
1	B	116	GLU
1	B	142	GLU
1	B	163	LEU
1	A	499	PRO
1	B	121	ASP
1	B	144	ASP
1	B	161	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	510/526 (97%)	493 (97%)	17 (3%)	33	63
1	B	492/526 (94%)	476 (97%)	16 (3%)	33	63
All	All	1002/1052 (95%)	969 (97%)	33 (3%)	33	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	88	THR
1	A	129	ASP
1	A	157	GLN
1	A	212	LEU
1	A	254	ASP
1	A	313	ARG
1	A	353	GLU
1	A	388	GLU
1	A	458	ILE
1	A	484	ARG
1	A	487	LYS
1	A	511	MET
1	A	567	ARG
1	A	569	SER

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Mol	Chain	Res	Type
1	A	629	VAL
1	A	635	ASN
1	B	82	VAL
1	B	88	THR
1	B	90	THR
1	B	119	LEU
1	B	192	LEU
1	B	211	ASN
1	B	212	LEU
1	B	252	ASP
1	B	267	LYS
1	B	301	MET
1	B	358	LYS
1	B	445	LEU
1	B	454	ARG
1	B	474	VAL
1	B	619	LEU
1	B	646	ASP

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

Mol	Chain	Res	Type
1	A	79	ASN
1	A	148	ASN
1	A	150	GLN
1	A	157	GLN
1	A	299	HIS
1	A	359	HIS
1	B	280	ASN
1	B	384	ASN
1	B	467	ASN
1	B	470	HIS
1	B	590	GLN
1	B	599	GLN
1	B	601	HIS
1	B	635	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	R1A	B	177	1	15,18,19	1.35	1 (6%)	15,27,29	4.09	8 (53%)
1	R1A	B	637	1	15,18,19	1.31	1 (6%)	15,27,29	4.12	8 (53%)
1	R1A	A	177	1	15,18,19	2.23	4 (26%)	15,27,29	4.99	8 (53%)
1	R1A	A	637	1	15,18,19	1.31	1 (6%)	15,27,29	4.09	8 (53%)

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
1	R1A	B	177	1	-	2/5/32/34	0/1/1/1
1	R1A	B	637	1	-	2/5/32/34	0/1/1/1
1	R1A	A	177	1	-	4/5/32/34	0/1/1/1
1	R1A	A	637	1	-	3/5/32/34	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	R1A	C2-N1	5.45	1.62	1.47
1	A	177	R1A	C5-C4	-4.84	1.43	1.50
1	B	177	R1A	CE-SD	-3.89	1.76	1.82
1	B	637	R1A	CE-SD	-3.88	1.76	1.82
1	A	637	R1A	CE-SD	-3.86	1.76	1.82
1	A	177	R1A	CB-CA	-3.17	1.45	1.53
1	A	177	R1A	C4-C3	2.87	1.35	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	R1A	C8-C2-N1	-10.23	83.49	109.91
1	A	177	R1A	C9-C2-N1	-9.50	85.36	109.91
1	A	177	R1A	CE-SD-SG	-8.95	93.95	103.62
1	B	637	R1A	C9-C2-N1	-7.58	90.33	109.91
1	A	637	R1A	C8-C2-N1	-7.58	90.33	109.91
1	B	637	R1A	C8-C2-N1	-7.57	90.34	109.91
1	B	177	R1A	C8-C2-N1	-7.57	90.35	109.91
1	A	637	R1A	C9-C2-N1	-7.56	90.38	109.91
1	B	177	R1A	C9-C2-N1	-7.55	90.40	109.91
1	A	637	R1A	C8-C2-C9	6.67	124.85	112.26
1	B	637	R1A	C8-C2-C9	6.67	124.85	112.26
1	B	177	R1A	C8-C2-C9	6.66	124.83	112.26
1	A	177	R1A	CB-SG-SD	-6.28	87.61	103.86
1	B	637	R1A	C5-C4-C3	-6.06	108.01	113.48
1	B	177	R1A	C5-C4-C3	-6.02	108.04	113.48
1	A	637	R1A	C5-C4-C3	-6.01	108.05	113.48
1	B	637	R1A	O1-N1-C5	-4.47	113.54	122.78
1	A	637	R1A	O1-N1-C5	-4.47	113.54	122.78
1	B	177	R1A	O1-N1-C5	-4.46	113.55	122.78
1	A	177	R1A	C8-C2-C9	4.39	120.55	112.26
1	A	177	R1A	CA-CB-SG	4.35	132.28	114.45
1	B	637	R1A	C7-C5-C4	-3.33	109.55	112.76
1	B	637	R1A	C6-C5-C4	-3.31	109.56	112.76
1	B	177	R1A	C6-C5-C4	-3.30	109.58	112.76
1	A	637	R1A	C7-C5-C4	-3.29	109.59	112.76
1	B	177	R1A	C7-C5-C4	-3.24	109.63	112.76
1	A	637	R1A	C6-C5-C4	-3.22	109.65	112.76
1	B	637	R1A	O1-N1-C2	2.80	128.57	122.78
1	B	177	R1A	O1-N1-C2	2.79	128.56	122.78
1	A	637	R1A	O1-N1-C2	2.78	128.53	122.78
1	A	177	R1A	O1-N1-C5	-2.62	117.37	122.78
1	A	177	R1A	CB-CA-C	-2.40	104.28	110.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	177	R1A	N-CA-CB-SG
1	A	177	R1A	C4-C3-CE-SD
1	B	177	R1A	C3-CE-SD-SG
1	A	637	R1A	CE-SD-SG-CB
1	A	637	R1A	C3-CE-SD-SG
1	A	177	R1A	CE-SD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	B	177	R1A	CE-SD-SG-CB
1	B	637	R1A	CA-CB-SG-SD
1	B	637	R1A	C4-C3-CE-SD
1	A	637	R1A	C4-C3-CE-SD
1	A	177	R1A	CA-CB-SG-SD

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	637	R1A	1	0
1	A	177	R1A	1	0
1	A	637	R1A	8	0

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	$\# Z > 2$
4	NAP	A	703	-	50,52,52	1.91	11 (22%)	71,80,80	1.79	15 (21%)
4	NAP	B	703	-	50,52,52	1.89	11 (22%)	71,80,80	1.80	17 (23%)
2	FMN	A	701	-	33,33,33	1.81	8 (24%)	48,50,50	1.62	10 (20%)
3	FAD	A	702	-	58,58,58	2.30	13 (22%)	85,89,89	1.96	17 (20%)
3	FAD	B	702	-	58,58,58	2.30	13 (22%)	85,89,89	1.97	16 (18%)
2	FMN	B	701	-	33,33,33	2.76	13 (39%)	48,50,50	1.65	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	-	-	9/35/67/67	0/5/5/5
4	NAP	B	703	-	-	12/35/67/67	0/5/5/5
2	FMN	A	701	-	-	4/18/18/18	0/3/3/3
3	FAD	A	702	-	-	5/34/50/50	0/6/6/6
3	FAD	B	702	-	-	4/34/50/50	0/6/6/6
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C8A-N7A	8.58	1.48	1.31
3	A	702	FAD	C8A-N7A	8.56	1.48	1.31
4	A	703	NAP	C3N-C7N	-7.50	1.39	1.50
4	B	703	NAP	C3N-C7N	-7.38	1.39	1.50
2	B	701	FMN	C8M-C8	-6.79	1.38	1.51
3	B	702	FAD	C8A-N9A	6.27	1.48	1.37
3	A	702	FAD	C8A-N9A	6.14	1.48	1.37
3	B	702	FAD	C7M-C7	-6.13	1.39	1.51
3	A	702	FAD	C8M-C8	-6.13	1.39	1.51
3	A	702	FAD	C7M-C7	-6.12	1.39	1.51
3	B	702	FAD	C8M-C8	-6.06	1.39	1.51
2	B	701	FMN	C10-N10	5.53	1.49	1.37
2	B	701	FMN	C4A-N5	5.52	1.42	1.30
2	B	701	FMN	C9-C9A	5.42	1.48	1.39
4	A	703	NAP	C2N-N1N	5.18	1.40	1.35
4	B	703	NAP	C2N-N1N	5.04	1.40	1.35
2	B	701	FMN	C9A-C5A	4.28	1.48	1.41
2	B	701	FMN	C9A-N10	4.23	1.48	1.41
2	A	701	FMN	C9A-C5A	4.20	1.47	1.41
2	B	701	FMN	C8-C7	3.98	1.50	1.40
2	A	701	FMN	C4-N3	-3.97	1.31	1.38
3	A	702	FAD	C9A-N10	-3.75	1.34	1.41
3	B	702	FAD	C9A-N10	-3.73	1.34	1.41
4	A	703	NAP	C2A-N1A	3.63	1.40	1.33
4	A	703	NAP	C2A-N3A	3.63	1.40	1.33
3	A	702	FAD	C10-N1	3.61	1.40	1.33
3	B	702	FAD	C10-N1	3.61	1.40	1.33
3	A	702	FAD	C2A-N1A	3.57	1.40	1.33
4	B	703	NAP	C2A-N1A	3.56	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C2A-N3A	3.55	1.40	1.33
4	B	703	NAP	C2A-N3A	3.54	1.40	1.33
3	B	702	FAD	C2A-N1A	3.53	1.40	1.33
3	A	702	FAD	C2A-N3A	3.53	1.40	1.33
2	B	701	FMN	C10-N1	3.53	1.40	1.33
2	B	701	FMN	C6-C5A	3.24	1.44	1.40
4	A	703	NAP	C5A-C4A	-3.07	1.33	1.39
3	A	702	FAD	C5A-N7A	-3.07	1.33	1.39
4	A	703	NAP	C5A-N7A	-3.06	1.33	1.39
4	B	703	NAP	C5A-N7A	-3.05	1.33	1.39
4	B	703	NAP	C5A-C4A	-3.04	1.33	1.39
3	A	702	FAD	C5A-C4A	-2.97	1.33	1.39
3	B	702	FAD	C5A-N7A	-2.96	1.33	1.39
3	B	702	FAD	C5A-C4A	-2.91	1.33	1.39
2	B	701	FMN	O2'-C2'	2.90	1.49	1.43
2	A	701	FMN	C2-N3	-2.88	1.32	1.39
3	B	702	FAD	C5X-N5	-2.73	1.34	1.39
4	B	703	NAP	O4D-C1D	2.71	1.44	1.40
2	A	701	FMN	C8-C7	2.68	1.47	1.40
4	B	703	NAP	C5A-C6A	-2.67	1.33	1.41
2	A	701	FMN	P-O3P	-2.66	1.44	1.54
3	B	702	FAD	C5A-C6A	-2.66	1.33	1.41
3	A	702	FAD	C5X-N5	-2.65	1.34	1.39
4	A	703	NAP	O4D-C1D	2.63	1.44	1.40
4	A	703	NAP	C5A-C6A	-2.62	1.33	1.41
3	A	702	FAD	C5A-C6A	-2.60	1.33	1.41
2	A	701	FMN	C5A-N5	-2.46	1.34	1.39
2	B	701	FMN	C4'-C3'	2.45	1.57	1.53
2	B	701	FMN	C6-C7	2.44	1.42	1.39
2	A	701	FMN	C9-C8	-2.43	1.36	1.39
4	B	703	NAP	C8A-N9A	-2.43	1.33	1.37
4	A	703	NAP	C8A-N9A	-2.42	1.33	1.37
2	A	701	FMN	C1'-C2'	-2.39	1.49	1.52
4	B	703	NAP	C6N-N1N	2.25	1.40	1.35
2	B	701	FMN	C7M-C7	2.21	1.55	1.51
4	A	703	NAP	C6N-N1N	2.18	1.40	1.35
4	B	703	NAP	C4A-N9A	-2.09	1.33	1.37
3	B	702	FAD	C4A-N9A	-2.04	1.33	1.37
4	A	703	NAP	C4A-N9A	-2.03	1.33	1.37
3	A	702	FAD	C4A-N9A	-2.02	1.33	1.37

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	FAD	N9A-C8A-N7A	-9.64	100.25	113.94
3	A	702	FAD	N9A-C8A-N7A	-9.16	100.94	113.94
3	B	702	FAD	N3A-C2A-N1A	-7.57	117.12	128.58
3	A	702	FAD	N3A-C2A-N1A	-7.22	117.65	128.58
4	A	703	NAP	N3A-C2A-N1A	-7.19	117.70	128.58
4	B	703	NAP	N3A-C2A-N1A	-7.16	117.74	128.58
3	A	702	FAD	C5A-C4A-N3A	-4.69	120.26	126.72
4	A	703	NAP	N9A-C8A-N7A	-4.68	107.30	113.94
4	B	703	NAP	N9A-C8A-N7A	-4.64	107.35	113.94
4	B	703	NAP	C4D-O4D-C1D	-4.60	105.71	109.92
3	B	702	FAD	C5A-C4A-N3A	-4.52	120.49	126.72
3	A	702	FAD	C5A-C4A-N9A	4.51	110.73	105.81
4	A	703	NAP	C5A-C4A-N3A	-4.27	120.84	126.72
2	A	701	FMN	C4-C4A-N5	4.23	124.05	118.21
4	B	703	NAP	C5A-C4A-N3A	-4.13	121.03	126.72
2	B	701	FMN	C9A-C5A-N5	3.91	126.61	122.45
3	B	702	FAD	C5A-C4A-N9A	3.65	109.78	105.81
3	B	702	FAD	C2A-N3A-C4A	3.62	120.67	111.83
3	A	702	FAD	C2A-N3A-C4A	3.58	120.58	111.83
2	A	701	FMN	C4A-C10-N10	3.57	121.59	116.48
2	B	701	FMN	C4'-C3'-C2'	-3.48	107.78	113.57
4	A	703	NAP	C5A-N7A-C8A	3.34	108.71	103.45
4	A	703	NAP	C2A-N3A-C4A	3.34	119.98	111.83
3	A	702	FAD	C5A-N7A-C8A	3.32	108.66	103.45
4	A	703	NAP	C3B-C2B-C1B	-3.31	96.47	102.81
4	B	703	NAP	C2A-N3A-C4A	3.31	119.91	111.83
3	B	702	FAD	C5A-C6A-N6A	-3.27	115.18	123.29
4	B	703	NAP	C5A-N7A-C8A	3.26	108.57	103.45
3	B	702	FAD	C4-N3-C2	-3.19	119.98	125.64
3	A	702	FAD	C4-N3-C2	-3.17	120.02	125.64
2	B	701	FMN	O3P-P-O5'	-3.15	98.46	106.67
3	B	702	FAD	C5A-N7A-C8A	3.13	108.38	103.45
2	B	701	FMN	O4-C4-N3	-3.00	114.47	120.11
3	A	702	FAD	C5A-C6A-N6A	-2.98	115.91	123.29
2	B	701	FMN	O4'-C4'-C3'	-2.97	102.29	109.25
2	B	701	FMN	C5A-C9A-N10	-2.96	115.29	117.97
4	A	703	NAP	C4D-O4D-C1D	-2.93	107.25	109.92
4	A	703	NAP	O4B-C1B-C2B	-2.84	101.69	106.59
3	A	702	FAD	C4A-N9A-C8A	2.84	108.72	105.74
3	A	702	FAD	C2B-C3B-C4B	-2.78	97.24	102.61
3	B	702	FAD	C10-C4X-N5	-2.75	119.20	124.81
2	A	701	FMN	O2-C2-N1	-2.75	117.24	121.80
4	B	703	NAP	C4A-N9A-C8A	2.71	108.59	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	NAP	C4A-C5A-N7A	-2.70	107.50	110.58
3	A	702	FAD	C4X-C4-N3	2.65	120.01	113.25
4	A	703	NAP	C5A-C6A-N6A	-2.64	116.74	123.29
3	A	702	FAD	O4-C4-C4X	-2.61	119.65	126.53
4	A	703	NAP	C4A-N9A-C8A	2.60	108.47	105.74
2	A	701	FMN	O4'-C4'-C5'	-2.59	104.27	109.99
4	B	703	NAP	C5A-C6A-N6A	-2.57	116.92	123.29
3	B	702	FAD	C4X-C4-N3	2.56	119.77	113.25
3	A	702	FAD	C10-C4X-N5	-2.55	119.60	124.81
4	B	703	NAP	C4A-C5A-N7A	-2.55	107.67	110.58
2	B	701	FMN	C8M-C8-C7	2.51	125.89	120.76
3	B	702	FAD	C4A-N9A-C8A	2.49	108.36	105.74
4	B	703	NAP	C6N-N1N-C2N	-2.45	119.79	121.88
4	A	703	NAP	C6A-C5A-C4A	2.43	120.50	117.18
2	B	701	FMN	O2P-P-O1P	2.40	120.20	110.83
3	A	702	FAD	C9A-C5X-N5	-2.39	119.91	122.45
4	B	703	NAP	C2D-C3D-C4D	-2.38	98.02	102.61
4	B	703	NAP	C6A-C5A-C4A	2.37	120.42	117.18
3	A	702	FAD	C6A-C5A-C4A	2.35	120.39	117.18
4	B	703	NAP	C3B-C2B-C1B	-2.33	98.34	102.81
2	B	701	FMN	C5A-N5-C4A	-2.31	114.35	118.09
4	A	703	NAP	N3A-C4A-N9A	2.29	131.06	127.17
3	B	702	FAD	C6A-C5A-C4A	2.28	120.30	117.18
2	A	701	FMN	C9A-N10-C10	-2.28	117.28	120.75
2	B	701	FMN	C9-C9A-N10	2.28	124.91	121.85
2	B	701	FMN	C7M-C7-C6	-2.25	115.60	119.57
3	B	702	FAD	C4X-C10-N10	2.25	119.70	116.48
3	B	702	FAD	C9A-C5X-N5	-2.24	120.07	122.45
3	B	702	FAD	O4-C4-C4X	-2.24	120.62	126.53
2	A	701	FMN	O3P-P-O2P	2.21	116.07	107.80
3	B	702	FAD	C4-C4X-C10	2.20	120.70	116.93
4	A	703	NAP	C3N-C7N-N7N	-2.19	115.03	117.74
2	B	701	FMN	C8M-C8-C9	-2.19	115.71	119.57
4	B	703	NAP	O4D-C4D-C3D	-2.18	100.82	105.15
4	A	703	NAP	C6N-N1N-C2N	-2.16	120.04	121.88
4	B	703	NAP	C3N-C7N-N7N	-2.16	115.07	117.74
2	A	701	FMN	O2'-C2'-C3'	2.15	114.28	109.25
2	A	701	FMN	C4A-C4-N3	2.13	118.69	113.25
2	A	701	FMN	C10-C4A-N5	-2.11	120.50	124.81
2	A	701	FMN	C4A-C10-N1	-2.08	119.50	124.59
3	A	702	FAD	C5A-C6A-N1A	2.04	122.70	117.51
3	A	702	FAD	C5X-C9A-N10	2.03	119.81	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	NAP	N3A-C4A-N9A	2.02	130.60	127.17
4	B	703	NAP	O4B-C1B-C2B	-2.00	103.14	106.59

There are no chirality outliers.

All (34) torsion outliers are listed below:

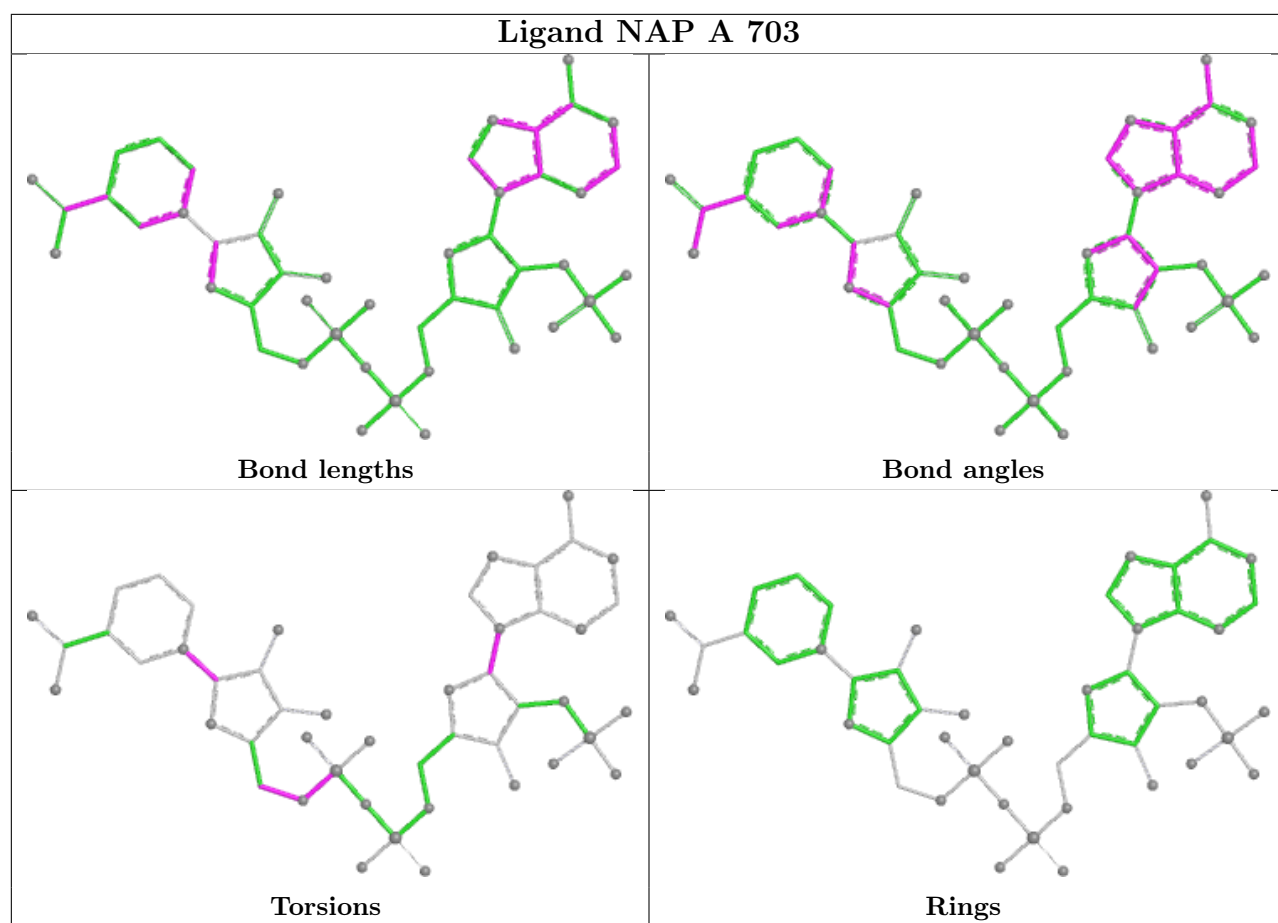
Mol	Chain	Res	Type	Atoms
2	A	701	FMN	C5'-O5'-P-O3P
3	A	702	FAD	C5'-O5'-P-O1P
4	A	703	NAP	C5D-O5D-PN-O3
4	A	703	NAP	C5D-O5D-PN-O1N
4	A	703	NAP	C5D-O5D-PN-O2N
4	A	703	NAP	C4D-C5D-O5D-PN
4	A	703	NAP	C2D-C1D-N1N-C6N
4	B	703	NAP	C4D-C5D-O5D-PN
4	B	703	NAP	O4D-C1D-N1N-C2N
4	B	703	NAP	O4D-C1D-N1N-C6N
4	B	703	NAP	C2D-C1D-N1N-C6N
4	A	703	NAP	C2B-C1B-N9A-C4A
4	B	703	NAP	C2B-C1B-N9A-C4A
4	B	703	NAP	C2B-C1B-N9A-C8A
4	A	703	NAP	C2B-C1B-N9A-C8A
2	A	701	FMN	C5'-O5'-P-O1P
4	B	703	NAP	PA-O3-PN-O5D
2	A	701	FMN	C5'-O5'-P-O2P
4	B	703	NAP	PN-O3-PA-O2A
3	A	702	FAD	C5'-O5'-P-O2P
3	A	702	FAD	C5'-O5'-P-O3P
4	A	703	NAP	C2D-C1D-N1N-C2N
2	A	701	FMN	C2'-C3'-C4'-C5'
3	A	702	FAD	PA-O3P-P-O2P
3	B	702	FAD	C4'-C5'-O5'-P
3	B	702	FAD	O2'-C2'-C3'-C4'
4	A	703	NAP	O4B-C1B-N9A-C8A
3	B	702	FAD	P-O3P-PA-O1A
4	B	703	NAP	PN-O3-PA-O1A
4	B	703	NAP	C3D-C4D-C5D-O5D
4	B	703	NAP	O4B-C1B-N9A-C8A
4	B	703	NAP	O4D-C4D-C5D-O5D
3	A	702	FAD	PA-O3P-P-O1P
3	B	702	FAD	P-O3P-PA-O2A

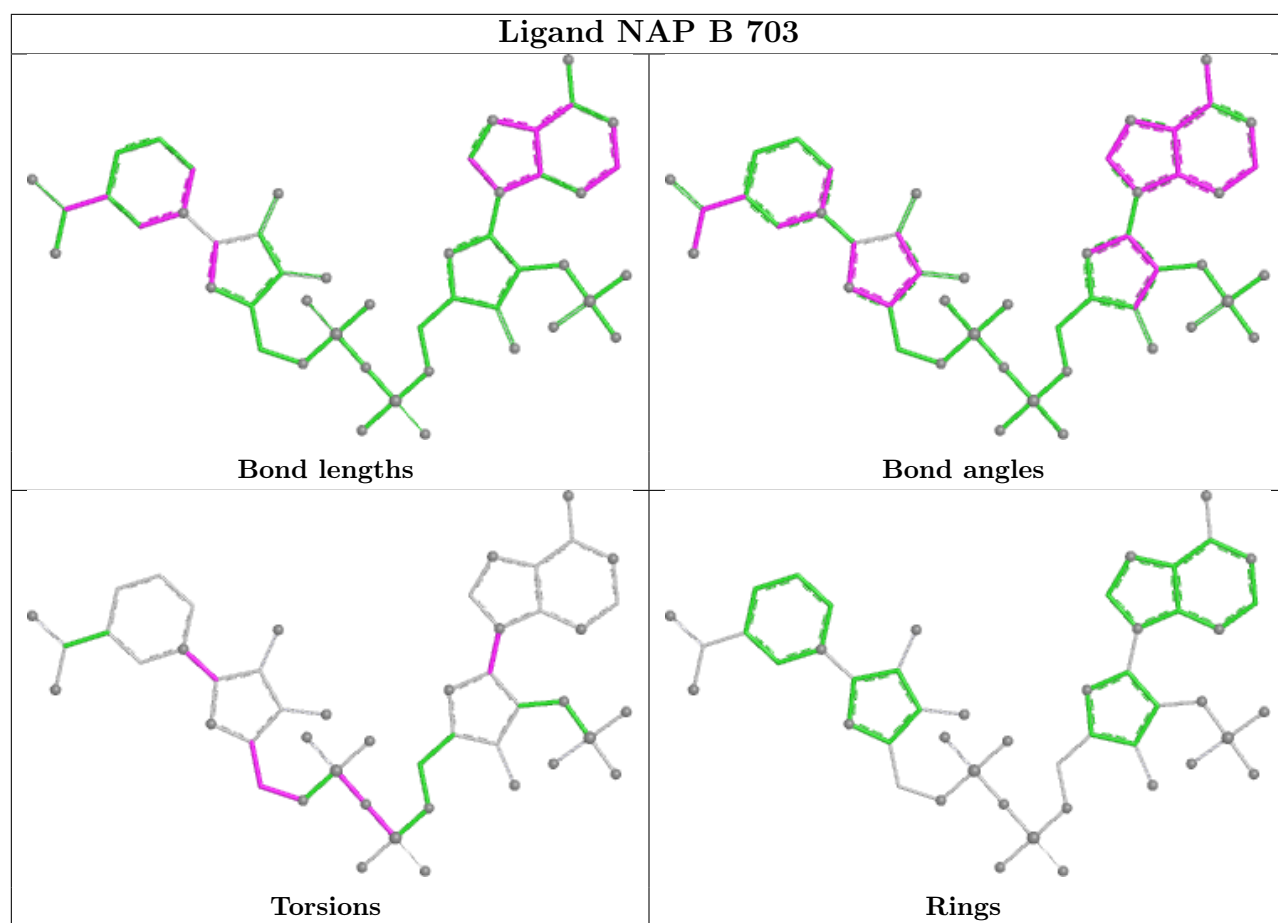
There are no ring outliers.

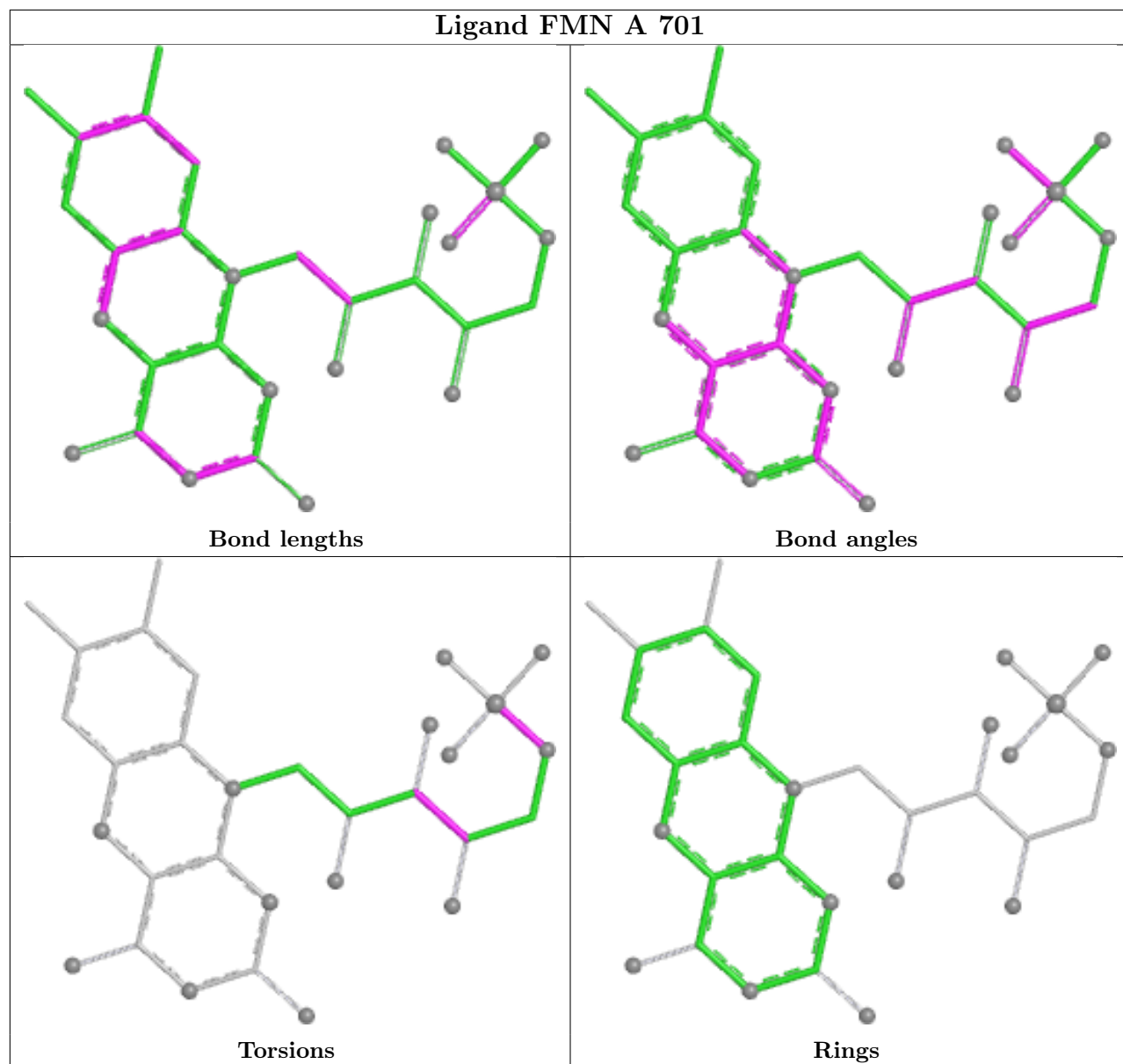
6 monomers are involved in 16 short contacts:

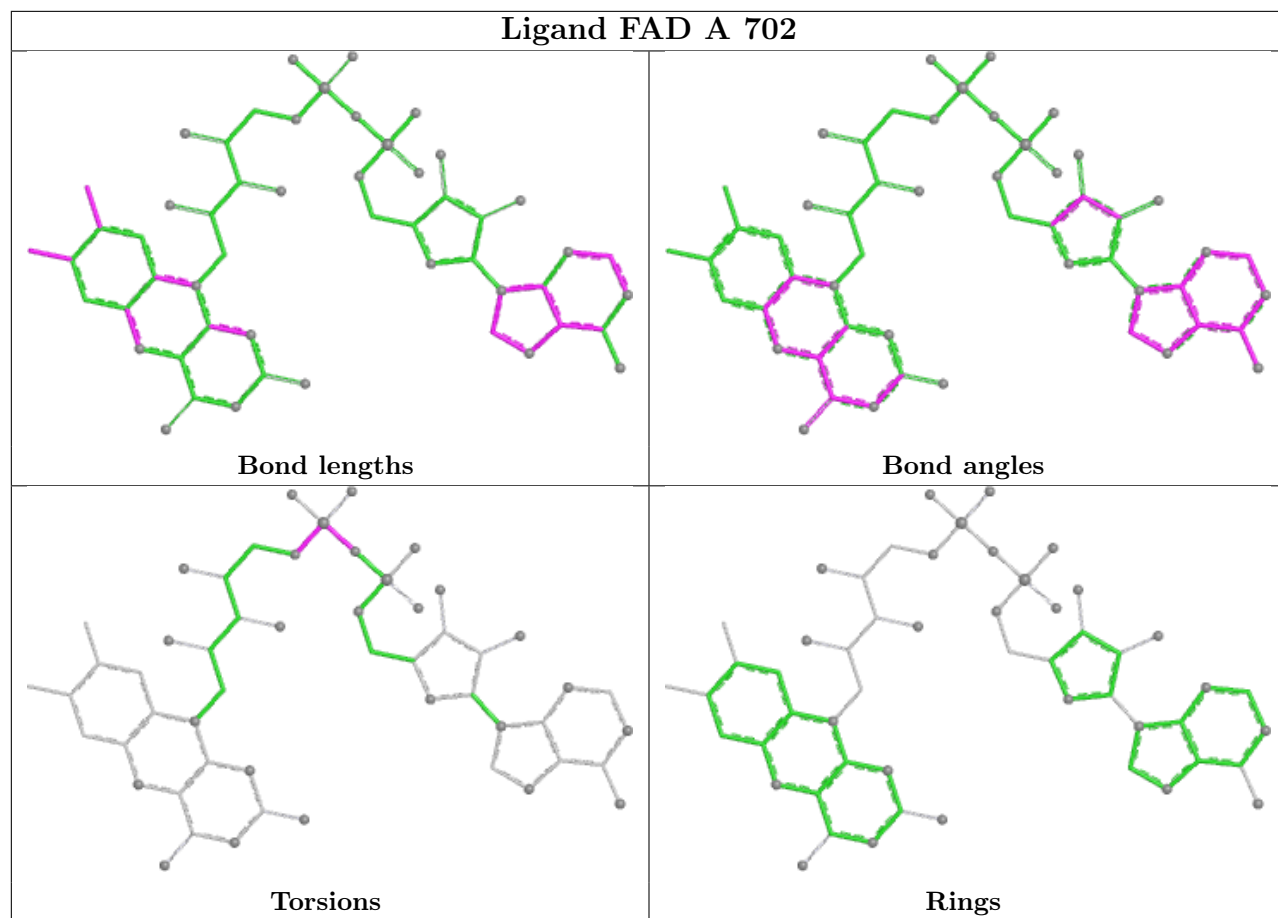
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	NAP	5	0
4	B	703	NAP	2	0
2	A	701	FMN	1	0
3	A	702	FAD	1	0
3	B	702	FAD	5	0
2	B	701	FMN	3	0

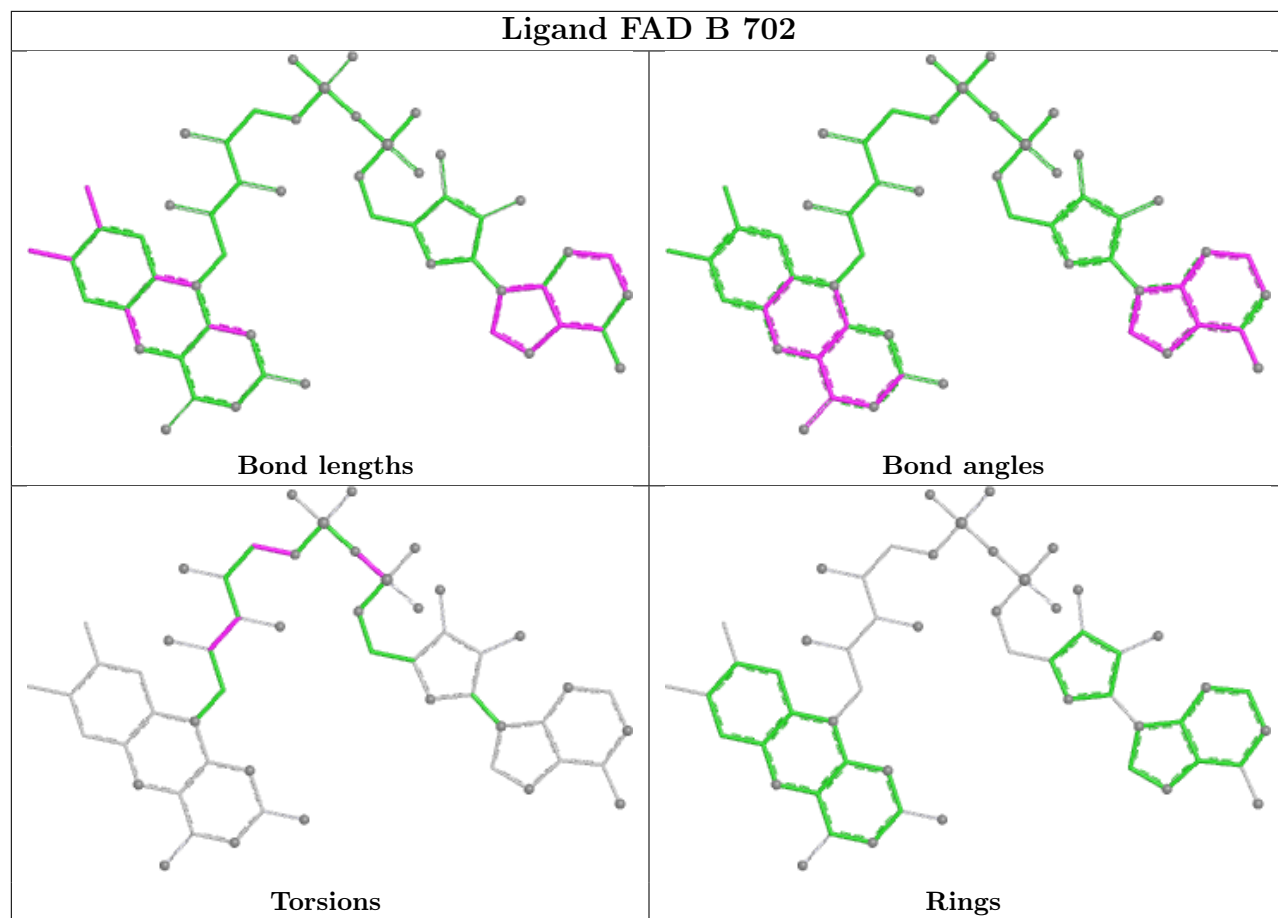
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

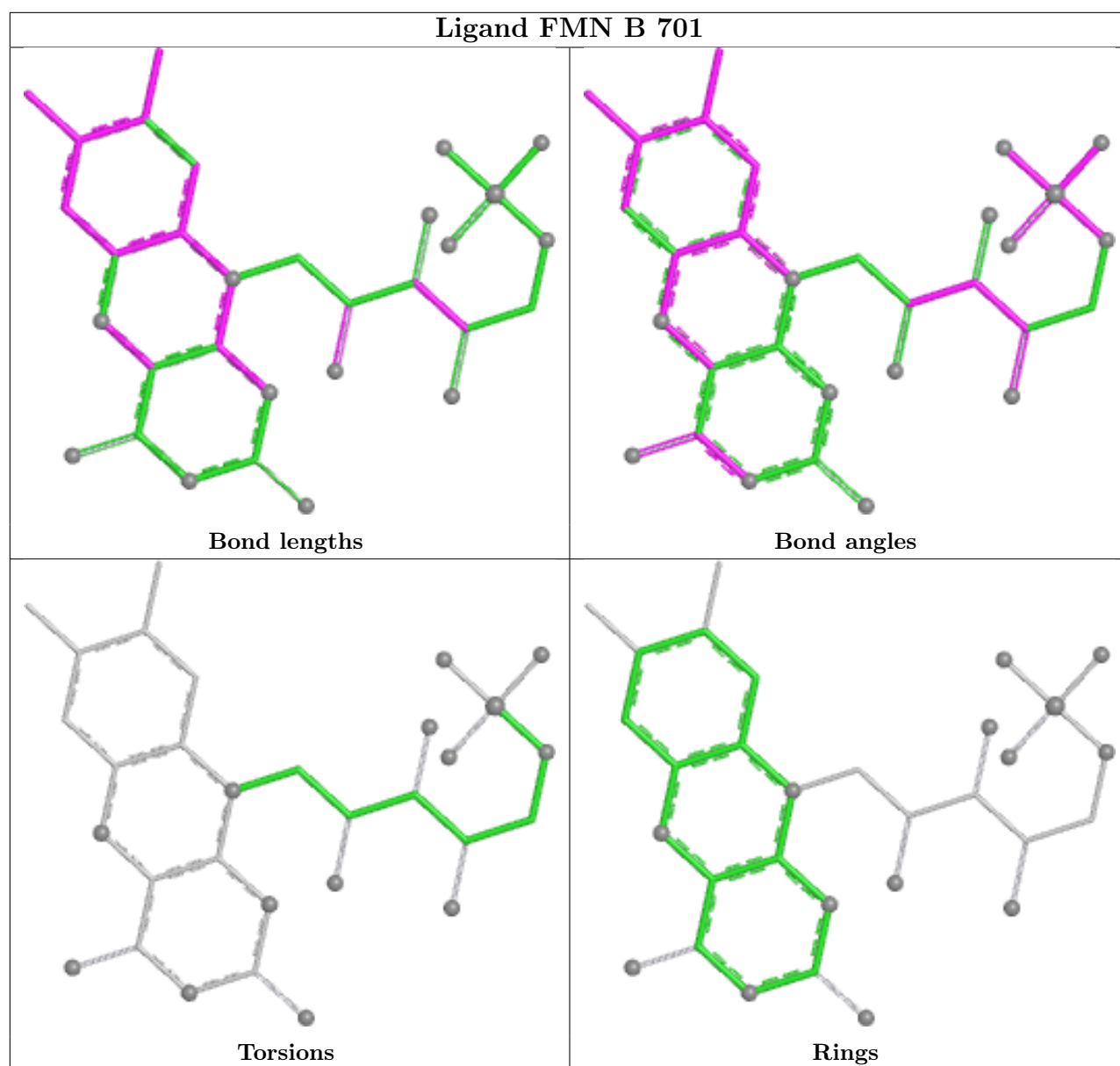












5.7 Other polymers [i](#)

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

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	607/622 (97%)	-0.03	7 (1%) 76 75	35, 57, 83, 108	0
1	B	603/622 (96%)	0.11	24 (3%) 42 38	34, 58, 108, 117	0
All	All	1210/1244 (97%)	0.04	31 (2%) 57 54	34, 58, 103, 117	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	PHE	4.1
1	B	64	VAL	3.8
1	B	233	VAL	3.3
1	A	178	TYR	3.0
1	A	236	THR	3.0
1	B	230	PHE	3.0
1	B	192	LEU	2.9
1	A	234	GLU	2.9
1	A	356	ASN	2.8
1	B	210	GLY	2.7
1	B	136	ALA	2.7
1	B	217	ILE	2.6
1	B	119	LEU	2.6
1	B	178	TYR	2.5
1	B	234	GLU	2.5
1	A	86	SER	2.4
1	A	240	SER	2.4
1	B	84	TYR	2.4
1	B	137	MET	2.3
1	B	104	ARG	2.3
1	B	166	VAL	2.3
1	B	163	LEU	2.3
1	B	240	SER	2.3
1	B	189	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	76	THR	2.2
1	B	161	VAL	2.2
1	B	160	ASP	2.2
1	B	188	VAL	2.2
1	A	500	ALA	2.1
1	B	500	ALA	2.1
1	B	101	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	R1A	B	177	18/19	0.59	0.18	103,121,123,123	0
1	R1A	A	637	18/19	0.67	0.28	69,109,113,114	0
1	R1A	B	637	18/19	0.71	0.24	63,94,98,99	0
1	R1A	A	177	18/19	0.72	0.16	104,130,132,133	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

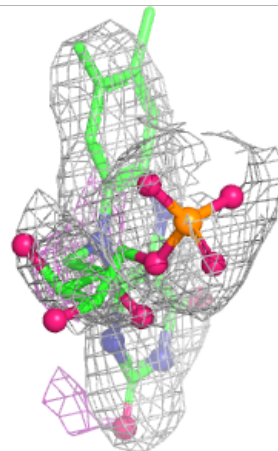
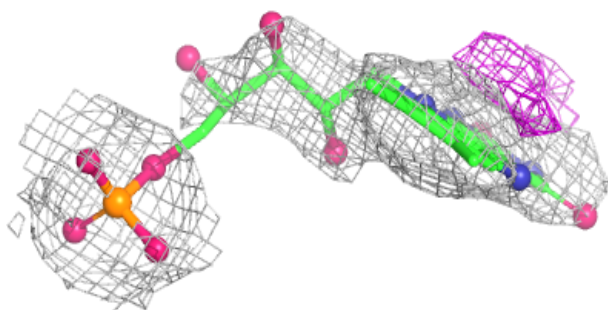
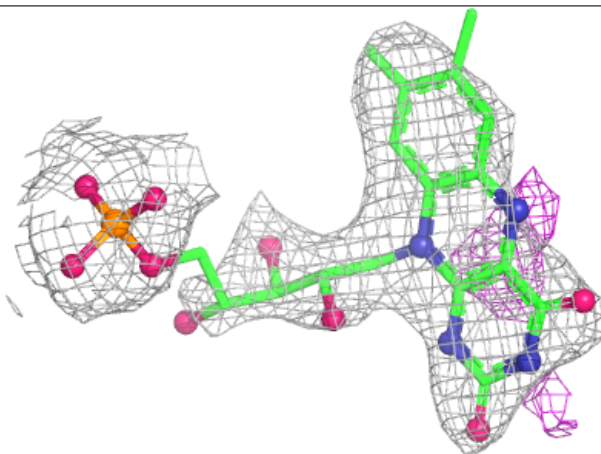
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	B	701	31/31	0.86	0.13	86,91,93,95	0
2	FMN	A	701	31/31	0.88	0.11	69,84,86,86	0
4	NAP	B	703	48/48	0.92	0.13	36,45,110,112	0
3	FAD	B	702	53/53	0.93	0.10	24,37,45,46	0
4	NAP	A	703	48/48	0.95	0.09	33,50,101,102	0
3	FAD	A	702	53/53	0.96	0.07	35,41,47,50	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.

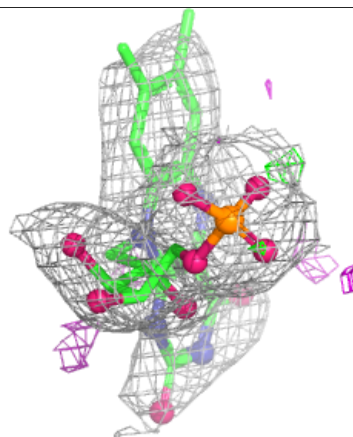
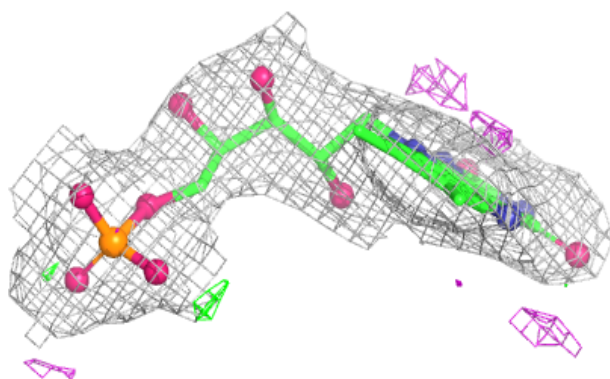
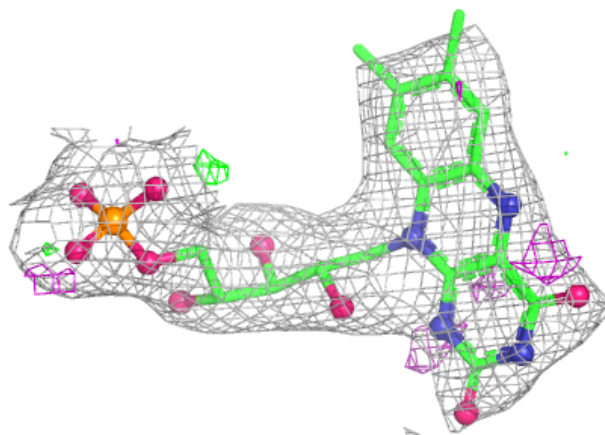
Electron density around FMN B 701:

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



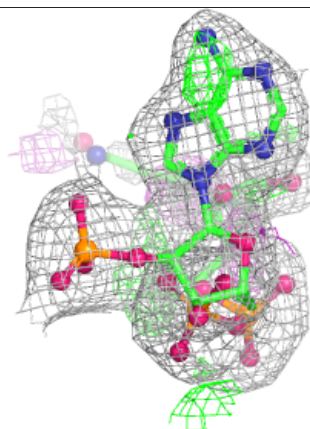
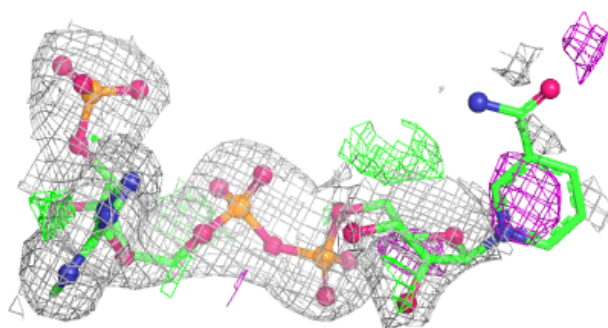
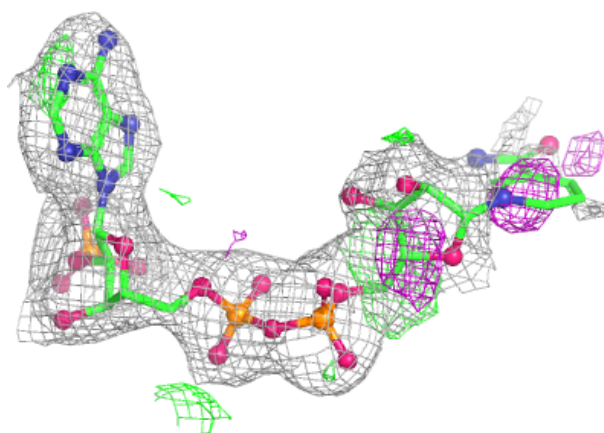
Electron density around FMN A 701:

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

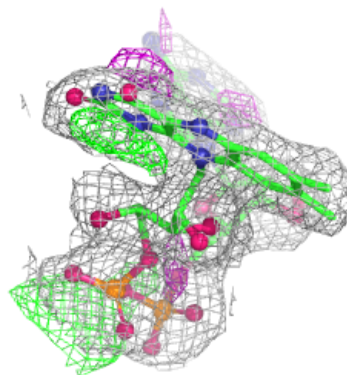
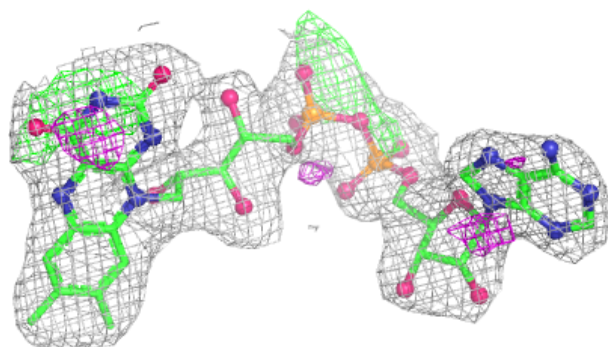
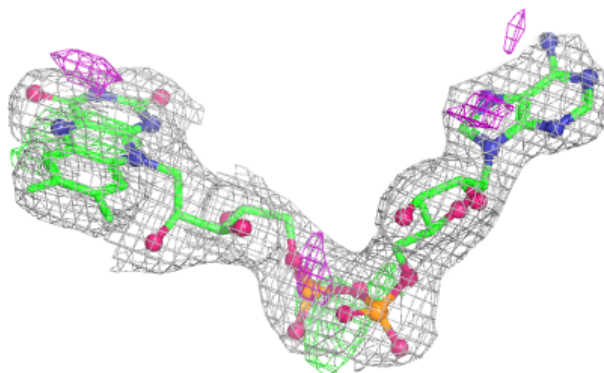


Electron density around NAP B 703:

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

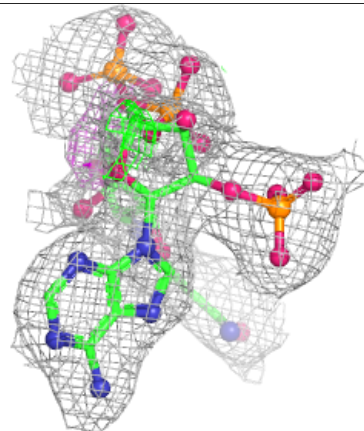
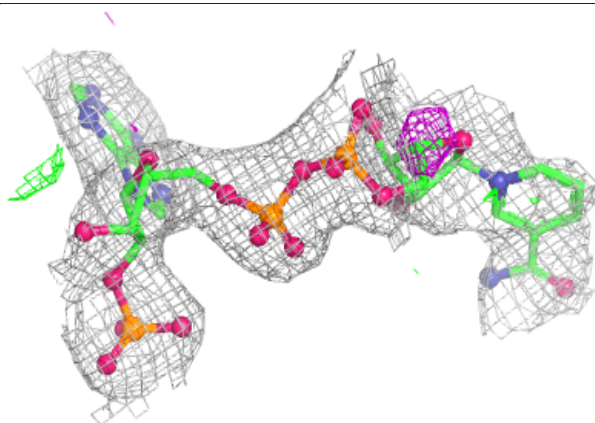
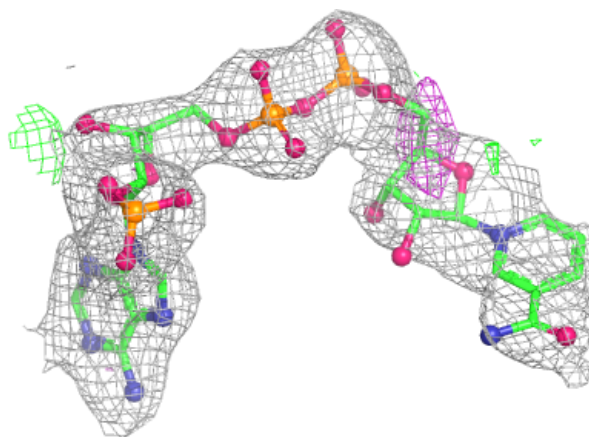
**Electron density around FAD B 702:**

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

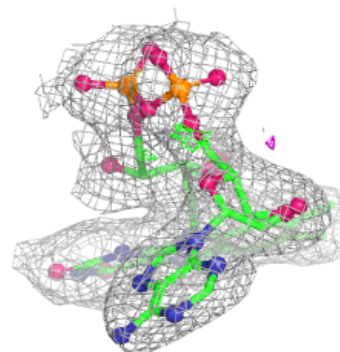
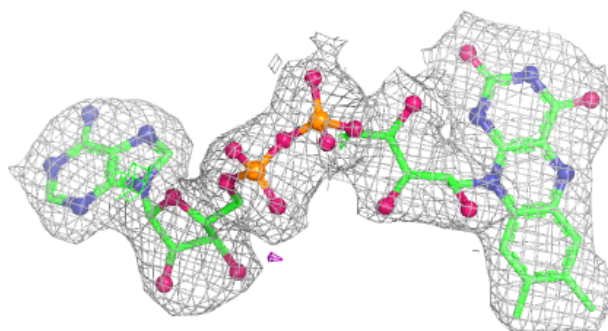
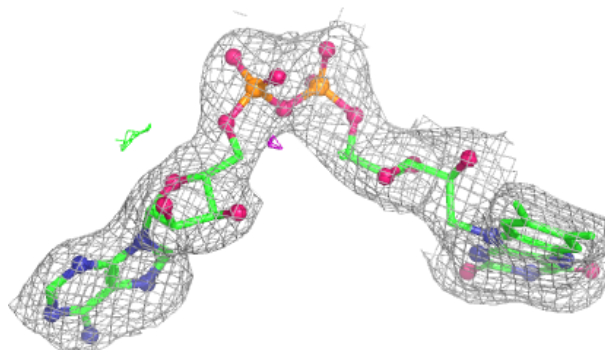


Electron density around NAP A 703:

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

**Electron density around FAD A 702:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.