Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 10:24 PM EDT

PDB ID	:	6NJR
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 (i) 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 (i)) were used in the production of this report:

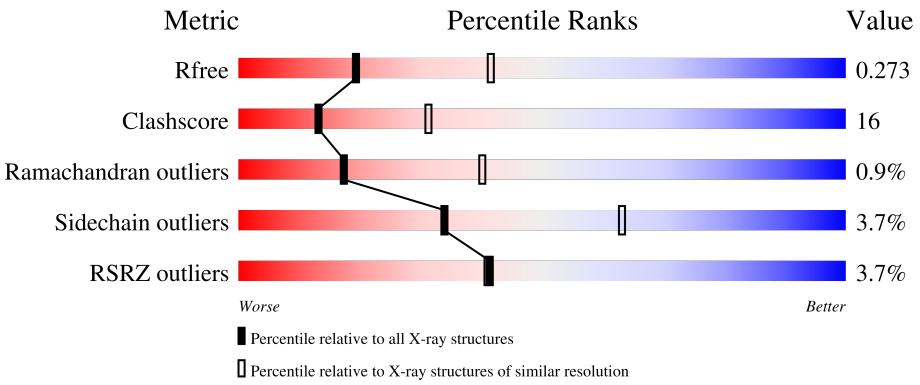
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	3% 67% 30% • •
1	B	622	5% 64% 32% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	R1A	A	177	-	-	-	X
1	R1A	A	637	-	-	X	X

2 Entry composition (i)

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.

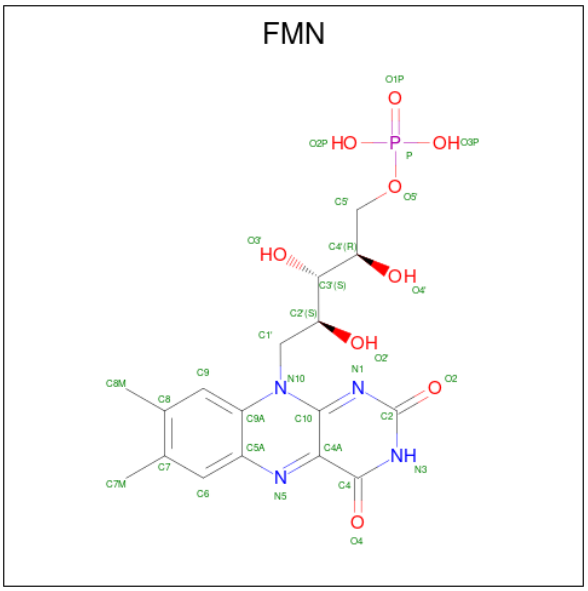
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

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

There are 18 discrepancies between the modelled and reference sequences:

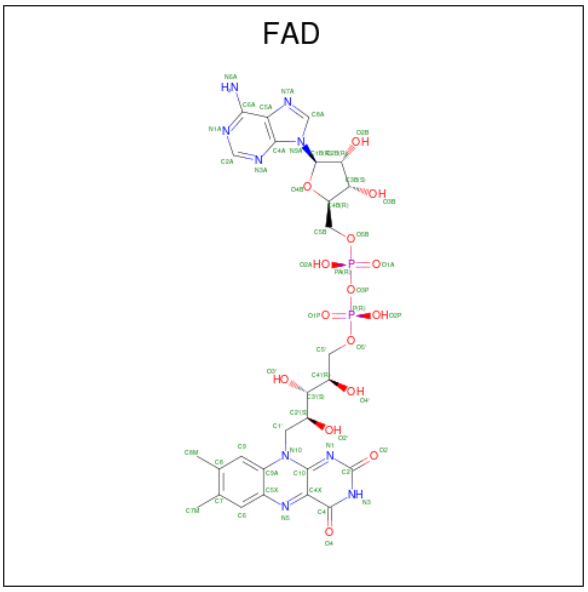
Chain	Residue	Modelled	Actual	Comment	Reference
A	136	ALA	CYS	engineered mutation	UNP P00388
A	177	R1A	THR	engineered mutation	UNP P00388
A	228	ALA	CYS	engineered mutation	UNP P00388
A	363	THR	CYS	engineered mutation	UNP P00388
A	445	LEU	CYS	engineered mutation	UNP P00388
A	472	THR	CYS	engineered mutation	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 (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

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



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

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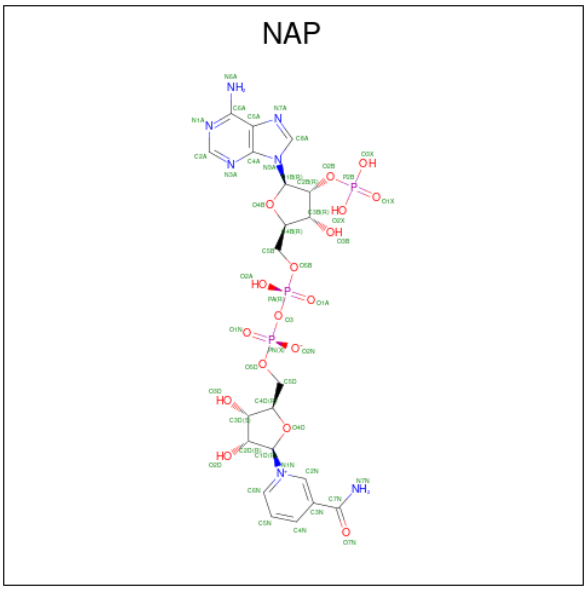
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	53	27	9	15	2	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
4	B	1	48	21	7	17	3	0	0

- Molecule 5 is water.

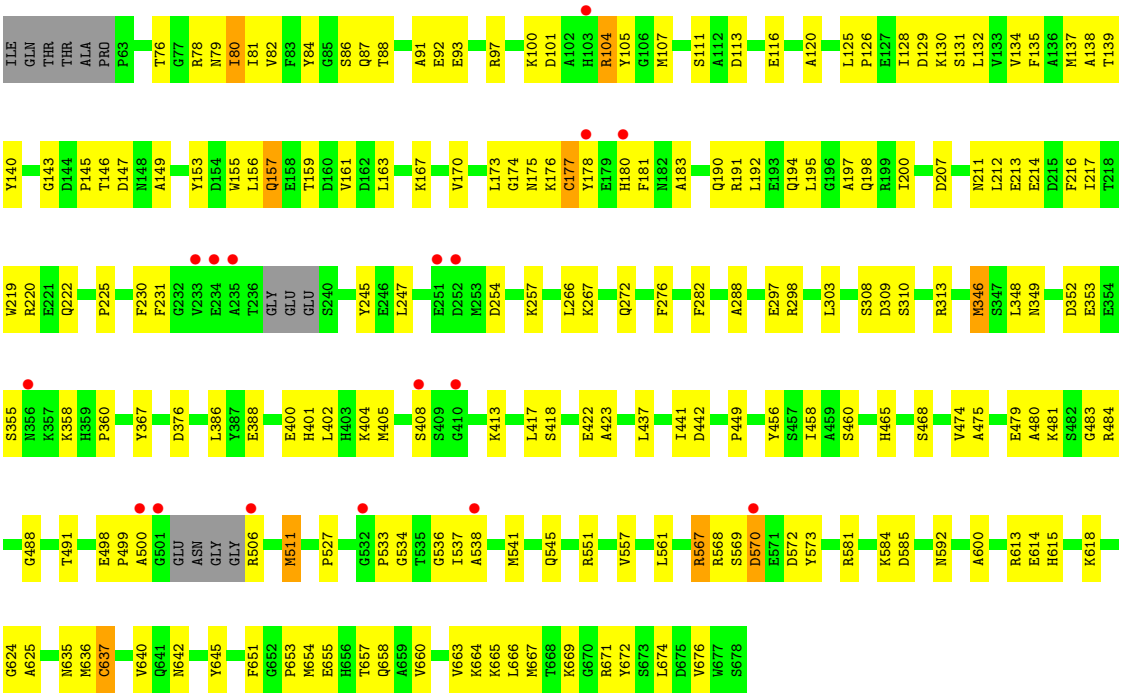
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	55	55	55	0	0
			Total	O		
5	B	52	52	52	0	0

3 Residue-property plots (i)

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

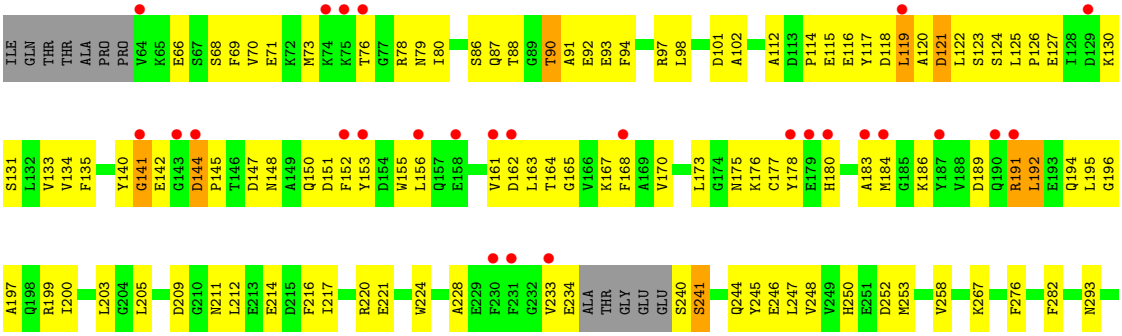
• Molecule 1: NADPH–cytochrome P450 reductase

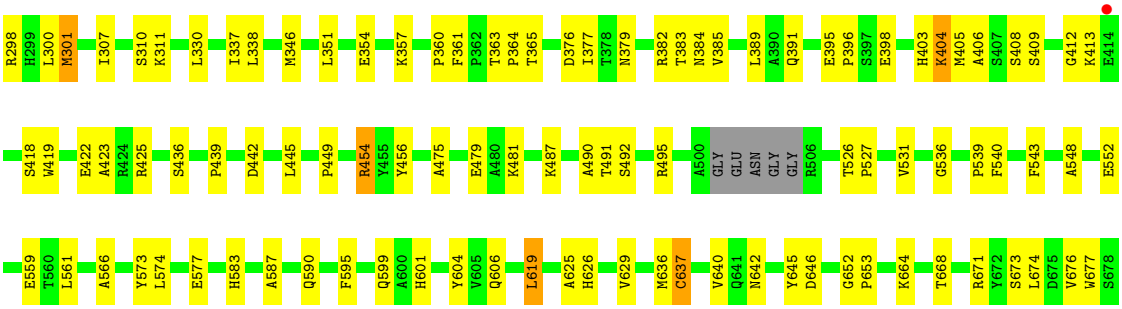
Chain A:



• Molecule 1: NADPH–cytochrome P450 reductase

Chain B:




R298 H299 L300 M301 I307 S310 K311 L330 I337 L338 M346 L351 E354 K357 P360 F361 P362 T363 P364 T365 D376 I377 T378 N379 R382 T383 N384 V385 L389 A390 Q391 E395 P396 S397 E398 H403 K404 M405 A406 S407 S408 S409 G412 K413 E414
S418 W419 E422 A423 R424 R425 S436 P439 D442 L445 P449 R454 Y455 Y456 A475 E479 A480 K481 K487 A490 T491 S492 R495 A500 GLY GLU ASN GLY GLY R506 T526 P527 V531 G536 P539 F540 F543 A548 E552
E559 T560 L561 A566 Y573 L574 E577 H583 A587 Q590 F595 Q599 A600 H601 Y604 V605 Q606 L619 A625 H626 V629 M636 C637 V640 Q641 N642 Y645 D646 G652 P653 K664 T668 R671 Y672 S673 L674 D675 V676 W677 S678

4 Data and refinement statistics (i)

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 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.9 (32.37-2.70) 98.0 (32.37-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 2.68Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.216 , 0.278 0.212 , 0.273	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)	0.32 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: R1A, NAP, FAD, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	0/4966	0.79	1/6719 (0.0%)
1	B	0.50	0/4886	0.76	0/6616
All	All	0.52	0/9852	0.77	1/13335 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	TYR	CB-CA-C	8.69	127.78	110.40

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	155	0
1	B	4810	0	4596	161	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	4	0
4	A	48	0	25	5	0
4	B	48	0	25	2	0
5	A	55	0	0	4	0
5	B	52	0	0	2	0
All	All	10069	0	9477	316	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 16.

All (316) 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: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:H72	1:A:676:VAL:CG2	2.06	0.86
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:A:637:R1A:C7	1:A:676:VAL:HG21	2.13	0.78
1:A:637:R1A:H73	1:A:676:VAL:CG2	2.12	0.77
1:B:186:LYS:HG2	1:B:203:LEU:HD21	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:86:SER:CB	1:A:91:ALA:HB3	2.11	0.74
1:A:637:R1A:H72	1:A:676:VAL:HG23	1.70	0.72
1:A:637:R1A:C7	1:A:676:VAL:HG23	2.18	0.72
1:A:637:R1A:H72	1:A:676:VAL:HG21	1.70	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
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:301:MET:HE1	1:B:495:ARG:HG3	1.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:120:ALA:C	1:B:122:LEU:H	2.07	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:A:176:LYS:C	1:A:178:TYR:H	2.01	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:B:276:PHE:CG	1:B:282:PHE:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:214:GLU:CG	1:A:417:LEU:HD21	2.37	0.53
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:168:PHE:CE2	1:B:192:LEU:HB2	2.44	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:70:VAL:HA	1:B:73:MET:HE3	1.90	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:A:665:LYS:NZ	1:A:669:LYS:HE3	2.25	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:A:637:R1A:H93	1:A:674:LEU:HD13	1.93	0.50
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:162:ASP:C	1:B:164:THR:H	2.15	0.50
1:B:240:SER:O	1:B:241:SER:CB	2.58	0.50
1:A:132:LEU:HD11	1:A:200:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:221:GLU:CD	1:B:408:SER:HB3	2.32	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
1:A:216:PHE:O	1:A:220:ARG:HB2	2.12	0.49
1:A:665:LYS:HZ1	1:A:669:LYS:HE3	1.77	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: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:159:THR:OG1	1:A:161:VAL:HG12	2.14	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:A:498:GLU:C	1:A:500:ALA:H	2.17	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: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:615:HIS:O	1:A:618:LYS:HB3	2.15	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:A:441:ILE:HG23	1:A:442:ASP:N	2.29	0.46
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:583:HIS:CE1	5:B:828:HOH:O	2.68	0.46
1:B:301:MET:HE3	1:B:301:MET:HB3	1.49	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: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:115:GLU:C	1:B:117:TYR:H	2.18	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:541:MET:O	1:A:545:GLN:HG3	2.15	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:B:164:THR:HA	1:B:196:GLY:HA3	1.98	0.45
1:B:301:MET:CE	1:B:495:ARG:HA	2.47	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: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:A:76:THR:HG22	1:A:78:ARG:NH1	2.32	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
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:498:GLU:C	1:A:500:ALA:N	2.70	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:GLN:C	1:A:225:PRO:HD2	2.38	0.43
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:120:ALA:HA	1:B:155:TRP:CE2	2.53	0.43
1:A:511:MET:SD	1:A:511:MET:C	2.97	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:B:577:GLU:CD	1:B:577:GLU:H	2.22	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:637:R1A:H93	1:A:674:LEU:CD1	2.49	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:A:346:MET:HG2	1:A:367:TYR:CE1	2.54	0.42
1:B:548:ALA:HB2	1:B:587:ALA:HB1	2.01	0.42
1:B:176:LYS:C	1:B:178:TYR:H	2.23	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:B:403:HIS:C	1:B:405:MET:H	2.22	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:GLU:C	1:A:298:ARG:HG3	2.40	0.41
1:A:534:GLY:C	1:A:536:GLY:H	2.24	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: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:B:636:MET:SD	1:B:636:MET:C	2.99	0.41
1:A:481:LYS:C	1:A:483:GLY:N	2.72	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: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:A:91:ALA:HB2	1:A:173:LEU:HD22	2.03	0.41
1:A:137:MET:HE1	1:A:149:ALA:HB1	2.03	0.41
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:A:572:ASP:OD1	1:A:572:ASP:N	2.54	0.40
1:B:677:TRP:CZ2	3:B:702:FAD:C4X	3.04	0.40
1:B:125:LEU:C	1:B:127:GLU:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:138:ALA:HA	1:A:173:LEU:O	2.21	0.40
1:A:178:TYR:CE2	1:A:637:R1A:H71	2.56	0.40
1:A:653:PRO:O	1:A:654:MET:HB3	2.21	0.40
1:B:68:SER:HB3	1:B:71:GLU:CD	2.42	0.40
1:B:140:TYR:O	1:B:141:GLY:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	601/622 (97%)	554 (92%)	45 (8%)	2 (0%)	41 66
1	B	597/622 (96%)	537 (90%)	51 (8%)	9 (2%)	10 26
All	All	1198/1244 (96%)	1091 (91%)	96 (8%)	11 (1%)	17 40

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	SER
1	B	66	GLU
1	B	141	GLY
1	A	104	ARG
1	B	116	GLU
1	B	142	GLU

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/526 (97%)	492 (96%)	18 (4%)	36	65
1	B	492/526 (94%)	473 (96%)	19 (4%)	32	61
All	All	1002/1052 (95%)	965 (96%)	37 (4%)	34	63

All (37) 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	147	ASP
1	A	157	GLN
1	A	212	LEU
1	A	254	ASP
1	A	313	ARG
1	A	346	MET
1	A	353	GLU
1	A	388	GLU
1	A	484	ARG
1	A	511	MET
1	A	567	ARG
1	A	569	SER
1	A	570	ASP
1	A	573	TYR
1	A	635	ASN

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Mol	Chain	Res	Type
1	B	88	THR
1	B	90	THR
1	B	119	LEU
1	B	144	ASP
1	B	151	ASP
1	B	191	ARG
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	346	MET
1	B	404	LYS
1	B	445	LEU
1	B	454	ARG
1	B	573	TYR
1	B	619	LEU
1	B	646	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	87	GLN
1	A	157	GLN
1	B	467	ASN
1	B	470	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	A	637	1	15,18,19	1.34	1 (6%)	15,27,29	4.19	8 (53%)
1	R1A	A	177	1	15,18,19	2.17	4 (26%)	15,27,29	4.91	7 (46%)
1	R1A	B	637	1	15,18,19	1.35	1 (6%)	15,27,29	4.20	8 (53%)
1	R1A	B	177	1	15,18,19	1.38	1 (6%)	15,27,29	4.19	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	A	637	1	-	3/5/32/34	0/1/1/1
1	R1A	A	177	1	-	4/5/32/34	0/1/1/1
1	R1A	B	637	1	-	2/5/32/34	0/1/1/1
1	R1A	B	177	1	-	2/5/32/34	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	-4.30	1.43	1.50
1	B	177	R1A	CE-SD	-4.06	1.76	1.81
1	B	637	R1A	CE-SD	-4.05	1.76	1.81
1	A	637	R1A	CE-SD	-4.03	1.76	1.81
1	A	177	R1A	CB-CA	-3.29	1.45	1.53
1	A	177	R1A	C4-C3	2.90	1.35	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	-8.72	93.95	103.67
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	B	637	R1A	C5-C4-C3	-7.20	108.01	113.64
1	B	177	R1A	C5-C4-C3	-7.15	108.04	113.64
1	A	637	R1A	C5-C4-C3	-7.14	108.05	113.64
1	A	637	R1A	C8-C2-C9	6.64	124.85	112.26
1	B	637	R1A	C8-C2-C9	6.64	124.85	112.26
1	B	177	R1A	C8-C2-C9	6.62	124.83	112.26
1	A	177	R1A	CB-SG-SD	-6.26	87.61	103.82
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	4.37	120.55	112.26
1	A	177	R1A	CA-CB-SG	4.15	132.28	114.55
1	B	637	R1A	C7-C5-C4	-3.12	109.55	112.78
1	B	637	R1A	C6-C5-C4	-3.10	109.56	112.78
1	B	177	R1A	C6-C5-C4	-3.09	109.58	112.78
1	A	637	R1A	C7-C5-C4	-3.08	109.59	112.78
1	B	177	R1A	C7-C5-C4	-3.04	109.63	112.78
1	A	637	R1A	C6-C5-C4	-3.02	109.65	112.78
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

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	A	637	R1A	CE-SD-SG-CB
1	A	177	R1A	CE-SD-SG-CB
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	B	177	R1A	C3-CE-SD-SG
1	A	637	R1A	C3-CE-SD-SG
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 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	637	R1A	12	0
1	A	177	R1A	1	0
1	B	637	R1A	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
2	FMN	A	701	-	33,33,33	1.77	8 (24%)	48,50,50	1.64	13 (27%)
4	NAP	A	703	-	45,52,52	1.91	8 (17%)	56,80,80	1.52	8 (14%)
4	NAP	B	703	-	45,52,52	1.89	9 (20%)	56,80,80	1.43	7 (12%)
3	FAD	B	702	-	53,58,58	2.12	11 (20%)	68,89,89	1.57	11 (16%)
3	FAD	A	702	-	53,58,58	2.13	11 (20%)	68,89,89	1.53	10 (14%)
2	FMN	B	701	-	33,33,33	2.73	13 (39%)	48,50,50	1.63	13 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	701	-	-	4/18/18/18	0/3/3/3
4	NAP	A	703	-	-	9/31/67/67	0/5/5/5
4	NAP	B	703	-	-	10/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	702	-	-	3/30/50/50	0/6/6/6
3	FAD	A	702	-	-	4/30/50/50	0/6/6/6
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C8A-N7A	7.56	1.48	1.34
3	A	702	FAD	C8A-N7A	7.53	1.48	1.34
4	A	703	NAP	C3N-C7N	-7.42	1.39	1.50
4	B	703	NAP	C3N-C7N	-7.30	1.39	1.50
2	B	701	FMN	C8M-C8	-6.36	1.38	1.51
2	B	701	FMN	C4A-N5	6.13	1.42	1.30
3	B	702	FAD	C7M-C7	-5.74	1.39	1.51
3	A	702	FAD	C8M-C8	-5.74	1.39	1.51
3	A	702	FAD	C7M-C7	-5.73	1.39	1.51
3	B	702	FAD	C8M-C8	-5.68	1.39	1.51
2	B	701	FMN	C10-N10	5.46	1.49	1.37
2	B	701	FMN	C9-C9A	5.39	1.48	1.39
4	A	703	NAP	C2A-N3A	5.13	1.40	1.32
3	B	702	FAD	C2A-N3A	5.05	1.40	1.32
4	B	703	NAP	C2A-N3A	5.04	1.40	1.32
3	A	702	FAD	C2A-N3A	5.03	1.40	1.32
4	A	703	NAP	C2N-N1N	4.69	1.40	1.35
4	B	703	NAP	C2N-N1N	4.57	1.40	1.35
2	B	701	FMN	C9A-N10	4.17	1.48	1.41
2	B	701	FMN	C9A-C5A	4.11	1.48	1.41
2	A	701	FMN	C9A-C5A	4.04	1.47	1.41
2	A	701	FMN	C4-N3	-4.00	1.31	1.38
2	B	701	FMN	C8-C7	3.87	1.50	1.40
3	A	702	FAD	C9A-N10	-3.68	1.34	1.41
3	B	702	FAD	C9A-N10	-3.66	1.34	1.41
3	A	702	FAD	C10-N1	3.57	1.40	1.33
3	B	702	FAD	C10-N1	3.57	1.40	1.33
2	B	701	FMN	C10-N1	3.49	1.40	1.33
4	A	703	NAP	C2A-N1A	3.48	1.40	1.33
3	A	702	FAD	C2A-N1A	3.43	1.40	1.33
4	B	703	NAP	C2A-N1A	3.42	1.40	1.33
3	B	702	FAD	C2A-N1A	3.39	1.40	1.33
2	B	701	FMN	C6-C5A	3.14	1.44	1.40
2	B	701	FMN	O2'-C2'	2.87	1.49	1.43
4	A	703	NAP	C5A-C4A	-2.77	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	NAP	C5A-C4A	-2.75	1.33	1.40
2	A	701	FMN	C2-N3	-2.74	1.32	1.39
3	A	702	FAD	C5A-C4A	-2.70	1.33	1.40
3	B	702	FAD	C5A-C4A	-2.66	1.33	1.40
4	B	703	NAP	C6A-C5A	-2.62	1.33	1.43
3	B	702	FAD	C5X-N5	-2.61	1.34	1.39
3	B	702	FAD	C6A-C5A	-2.61	1.33	1.43
2	A	701	FMN	C8-C7	2.61	1.47	1.40
4	A	703	NAP	C6A-C5A	-2.58	1.33	1.43
2	A	701	FMN	P-O3P	-2.58	1.44	1.54
3	A	702	FAD	C6A-C5A	-2.57	1.33	1.43
3	A	702	FAD	C5X-N5	-2.54	1.34	1.39
4	B	703	NAP	O4D-C1D	2.42	1.44	1.41
2	A	701	FMN	C1'-C2'	-2.37	1.49	1.52
2	A	701	FMN	C5A-N5	-2.36	1.34	1.39
4	A	703	NAP	O4D-C1D	2.34	1.44	1.41
2	B	701	FMN	C6-C7	2.30	1.42	1.39
3	A	702	FAD	O4B-C1B	2.27	1.44	1.41
2	B	701	FMN	C4'-C3'	2.25	1.57	1.53
2	A	701	FMN	C9-C8	-2.23	1.36	1.39
4	B	703	NAP	C6N-N1N	2.07	1.40	1.35
2	B	701	FMN	C7M-C7	2.06	1.55	1.51
4	B	703	NAP	O4B-C1B	2.04	1.43	1.41
3	B	702	FAD	O4B-C1B	2.03	1.43	1.41
4	A	703	NAP	C6N-N1N	2.00	1.40	1.35

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	FAD	N3A-C2A-N1A	-7.39	117.12	128.68
3	A	702	FAD	N3A-C2A-N1A	-7.05	117.65	128.68
4	A	703	NAP	N3A-C2A-N1A	-7.03	117.70	128.68
4	B	703	NAP	N3A-C2A-N1A	-7.00	117.74	128.68
2	A	701	FMN	C4-C4A-N5	4.09	124.05	118.23
2	B	701	FMN	C9A-C5A-N5	3.84	126.61	122.43
3	B	702	FAD	P-O3P-PA	-3.74	119.98	132.83
2	A	701	FMN	C4A-C10-N10	3.49	121.59	116.48
4	A	703	NAP	C3B-C2B-C1B	-3.41	96.47	102.89
3	B	702	FAD	C5A-C6A-N6A	-3.40	115.18	120.35
3	A	702	FAD	P-O3P-PA	-3.19	121.89	132.83
2	B	701	FMN	P-O5'-C5'	3.18	127.05	118.30
2	B	701	FMN	O3P-P-O5'	-3.11	98.46	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	FAD	C4-N3-C2	-3.06	119.98	125.64
3	A	702	FAD	C4-N3-C2	-3.05	120.02	125.64
2	A	701	FMN	O2'-C2'-C1'	-3.04	102.45	109.80
2	B	701	FMN	O4-C4-N3	-2.94	114.47	120.12
3	A	702	FAD	C5A-C6A-N6A	-2.92	115.91	120.35
4	A	703	NAP	O4B-C1B-C2B	-2.82	101.69	106.59
2	B	701	FMN	O4'-C4'-C3'	-2.80	102.29	109.10
3	A	702	FAD	C2B-C3B-C4B	-2.78	97.24	102.64
2	A	701	FMN	O2-C2-N1	-2.77	117.24	121.83
3	A	702	FAD	C4X-C4-N3	2.69	120.01	113.19
2	B	701	FMN	C4'-C3'-C2'	-2.69	107.78	113.36
3	B	702	FAD	C10-C4X-N5	-2.67	119.20	124.86
4	A	703	NAP	C3D-C2D-C1D	-2.62	97.03	100.98
3	A	702	FAD	O4-C4-C4X	-2.62	119.65	126.60
3	B	702	FAD	C4X-C4-N3	2.59	119.77	113.19
2	B	701	FMN	C5A-C9A-N10	-2.58	115.29	117.95
2	B	701	FMN	C8M-C8-C7	2.51	125.89	120.74
2	A	701	FMN	O4'-C4'-C5'	-2.51	104.27	109.92
3	A	702	FAD	C10-C4X-N5	-2.48	119.60	124.86
2	B	701	FMN	O2P-P-O1P	2.43	120.20	110.68
4	B	703	NAP	C3B-C2B-C1B	-2.42	98.34	102.89
4	B	703	NAP	C6N-N1N-C2N	-2.39	119.79	121.97
4	B	703	NAP	C2D-C3D-C4D	-2.38	98.02	102.64
4	A	703	NAP	C5A-C6A-N6A	-2.38	116.74	120.35
3	B	702	FAD	C4-C4X-C10	2.33	120.70	116.79
3	A	702	FAD	C9A-C5X-N5	-2.32	119.91	122.43
2	B	701	FMN	C9-C9A-N10	2.28	124.91	121.84
4	A	703	NAP	C3N-C7N-N7N	-2.26	115.03	117.75
4	B	703	NAP	C5A-C6A-N6A	-2.26	116.92	120.35
2	A	701	FMN	C4A-C10-N1	-2.25	119.50	124.73
3	B	702	FAD	O4-C4-C4X	-2.25	120.62	126.60
4	A	703	NAP	O4D-C1D-C2D	-2.24	103.65	106.93
2	A	701	FMN	C9A-N10-C10	-2.24	117.28	120.77
2	B	701	FMN	C5A-N5-C4A	-2.24	114.35	118.07
4	B	703	NAP	C3N-C7N-N7N	-2.23	115.07	117.75
2	A	701	FMN	O3P-P-O2P	2.21	116.07	107.64
3	B	702	FAD	C4X-C10-N10	2.20	119.70	116.48
4	B	703	NAP	O4D-C4D-C3D	-2.17	100.82	105.11
3	B	702	FAD	C9A-C5X-N5	-2.17	120.07	122.43
2	A	701	FMN	C4A-C4-N3	2.16	118.69	113.19
3	B	702	FAD	C4X-C10-N1	-2.15	119.73	124.73
2	A	701	FMN	O2'-C2'-C3'	2.13	114.28	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	NAP	C6N-N1N-C2N	-2.12	120.04	121.97
2	B	701	FMN	C7M-C7-C6	-2.10	115.60	119.49
3	A	702	FAD	C4-C4X-C10	2.08	120.28	116.79
2	A	701	FMN	C10-C4A-N5	-2.05	120.50	124.86
2	B	701	FMN	C8M-C8-C9	-2.04	115.71	119.49
2	A	701	FMN	C10-N1-C2	2.03	120.97	116.90
2	A	701	FMN	O2P-P-O1P	2.00	118.51	110.68

There are no chirality outliers.

All (30) 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
3	A	702	FAD	C5'-O5'-P-O3P
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
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	B	702	FAD	C4'-C5'-O5'-P
4	B	703	NAP	O4D-C4D-C5D-O5D
3	A	702	FAD	PA-O3P-P-O2P
3	B	702	FAD	O2'-C2'-C3'-C4'
4	B	703	NAP	C3D-C4D-C5D-O5D
4	A	703	NAP	C2B-O2B-P2B-O1X
2	A	701	FMN	C2'-C3'-C4'-C5'
4	A	703	NAP	C2B-O2B-P2B-O2X
4	A	703	NAP	C5D-O5D-PN-O3
4	A	703	NAP	C2D-C1D-N1N-C2N
4	B	703	NAP	C5D-O5D-PN-O3
3	B	702	FAD	P-O3P-PA-O1A
4	B	703	NAP	PN-O3-PA-O1A
4	A	703	NAP	O4D-C4D-C5D-O5D

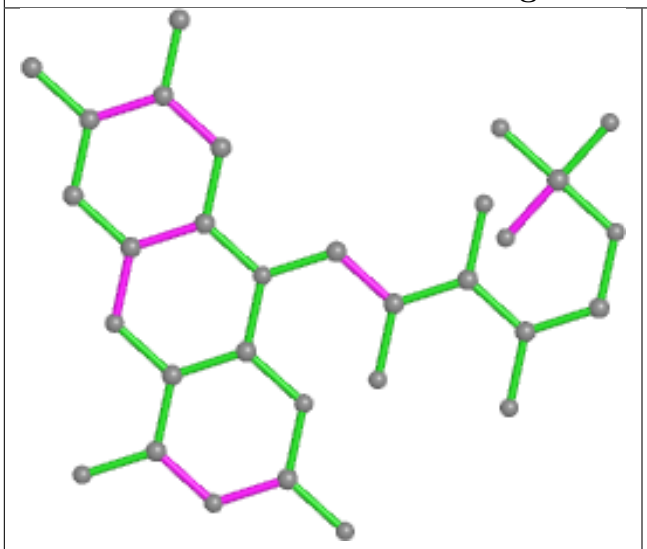
There are no ring outliers.

6 monomers are involved in 15 short contacts:

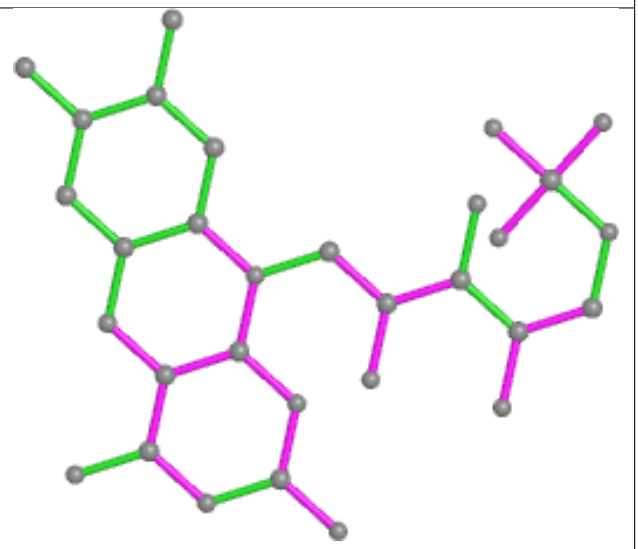
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FMN	1	0
4	A	703	NAP	5	0
4	B	703	NAP	2	0
3	B	702	FAD	4	0
3	A	702	FAD	1	0
2	B	701	FMN	3	0

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 then 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.

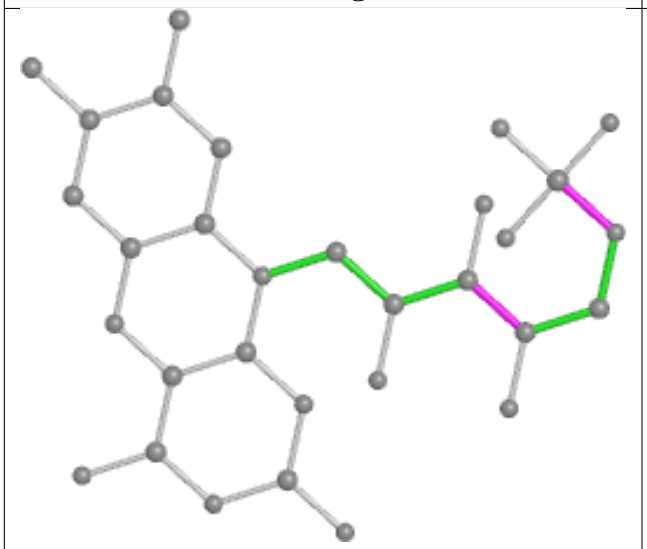
Ligand FMN A 701



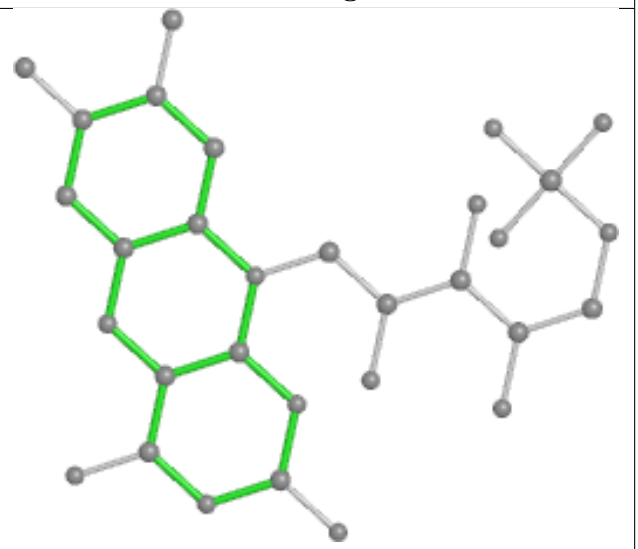
Bond lengths



Bond angles

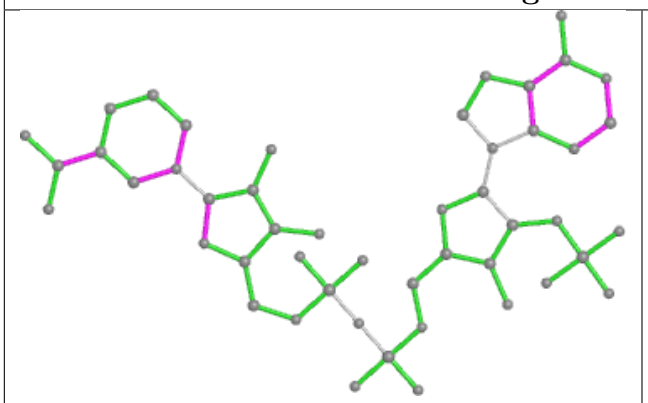


Torsions

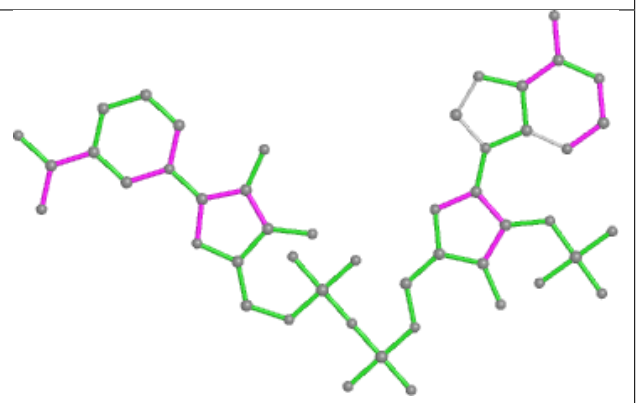


Rings

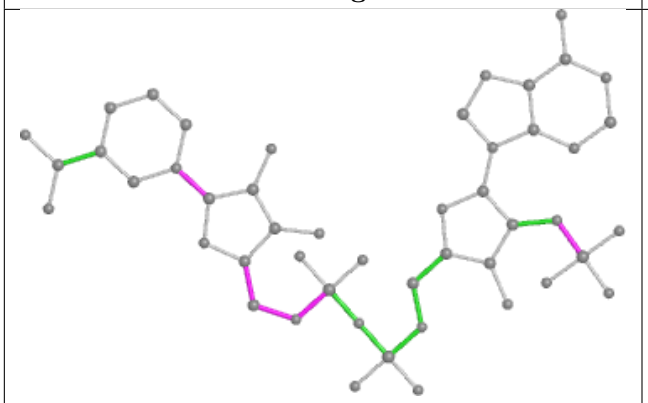
Ligand NAP A 703



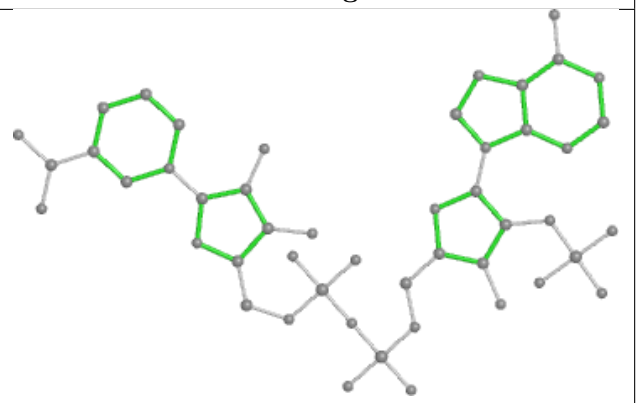
Bond lengths



Bond angles

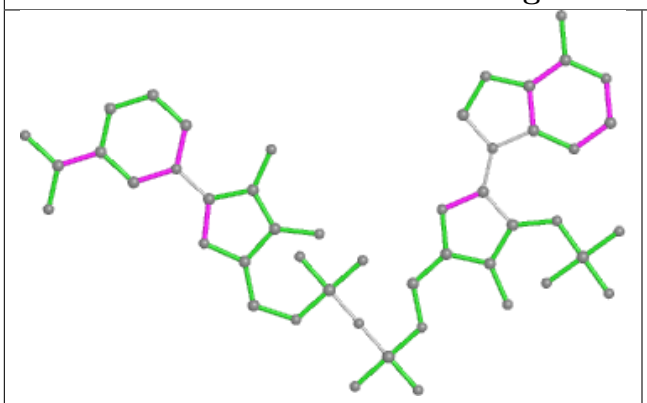


Torsions

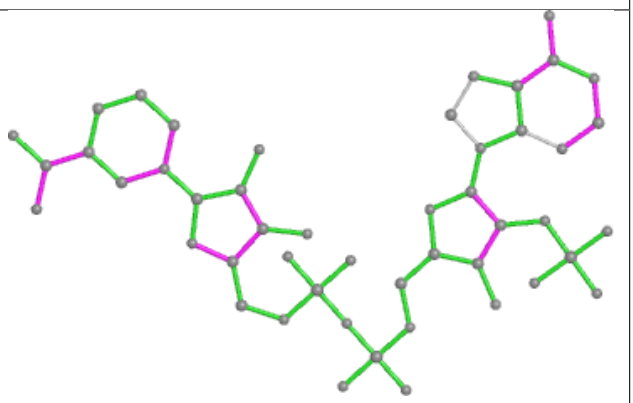


Rings

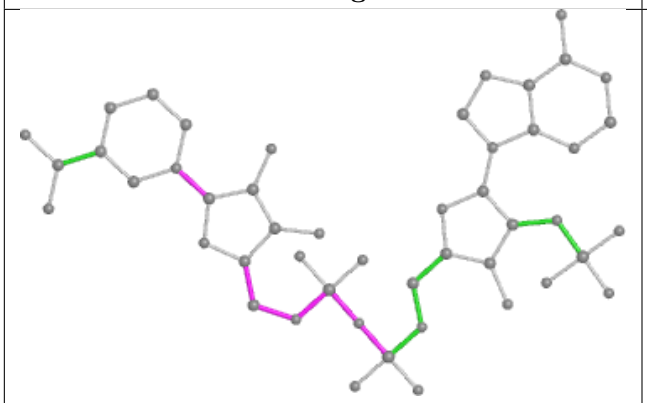
Ligand NAP B 703



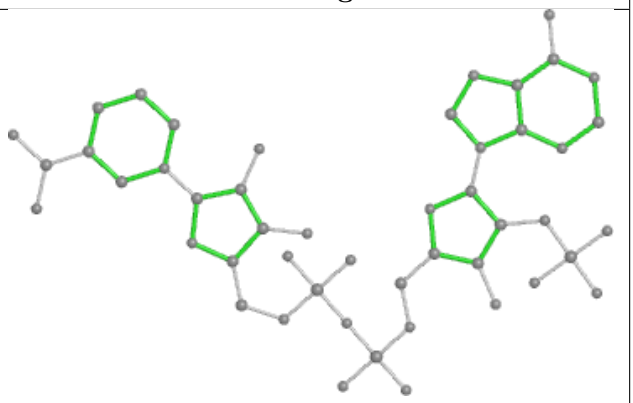
Bond lengths



Bond angles

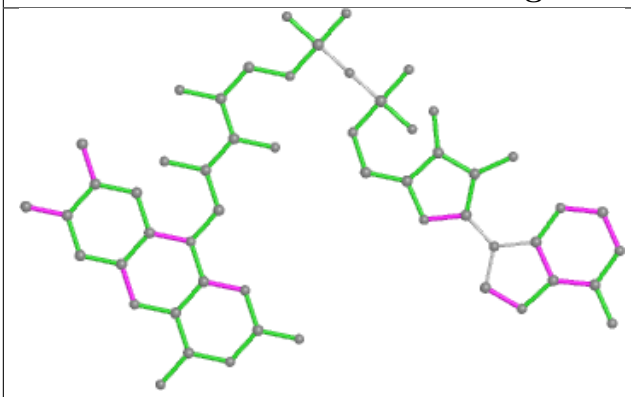


Torsions

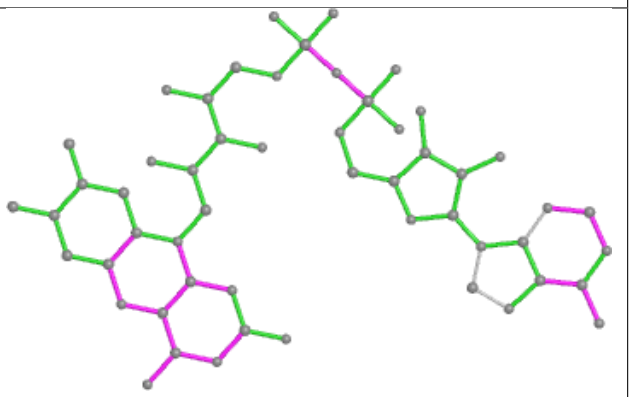


Rings

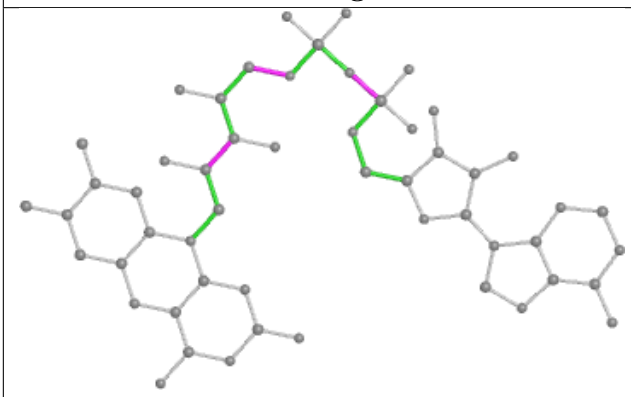
Ligand FAD B 702



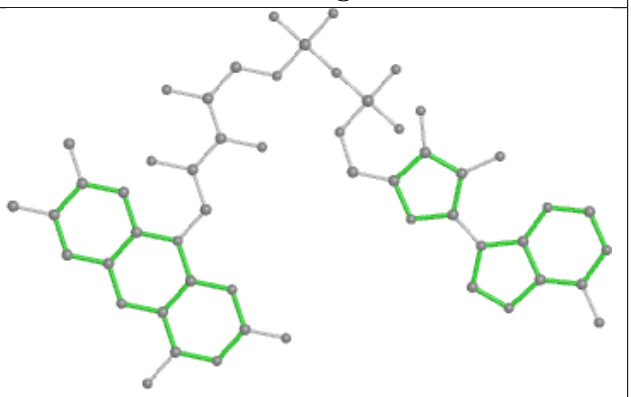
Bond lengths



Bond angles

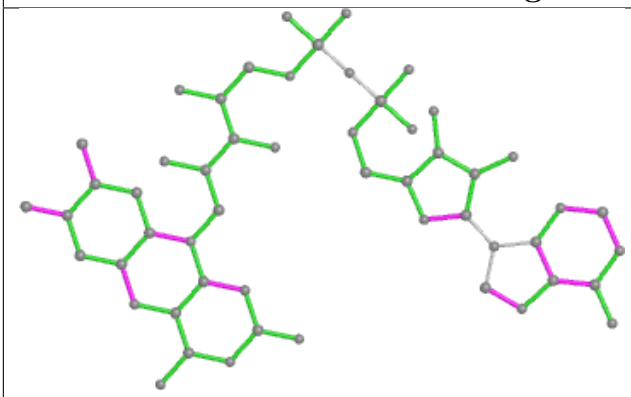


Torsions

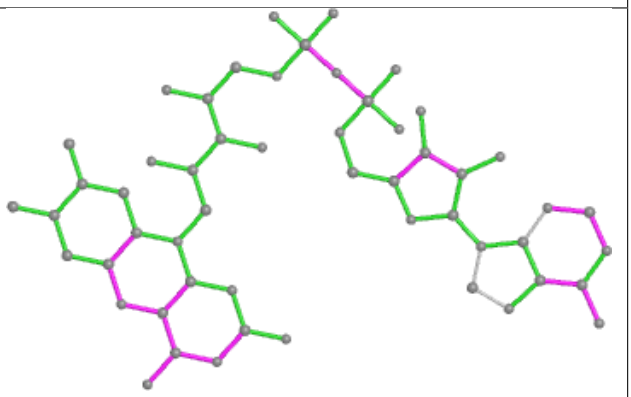


Rings

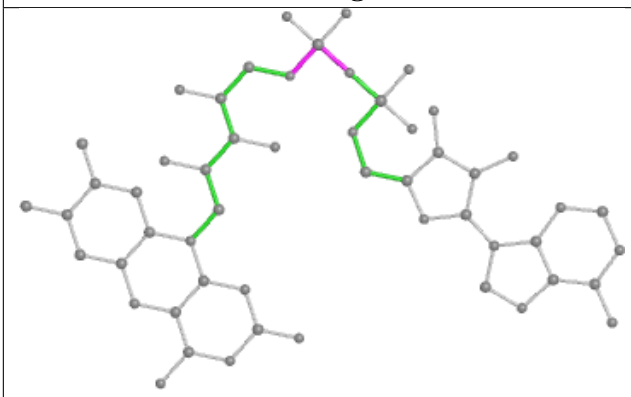
Ligand FAD A 702



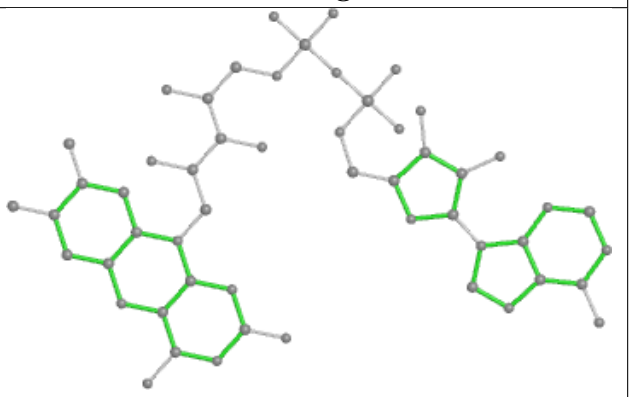
Bond lengths



Bond angles

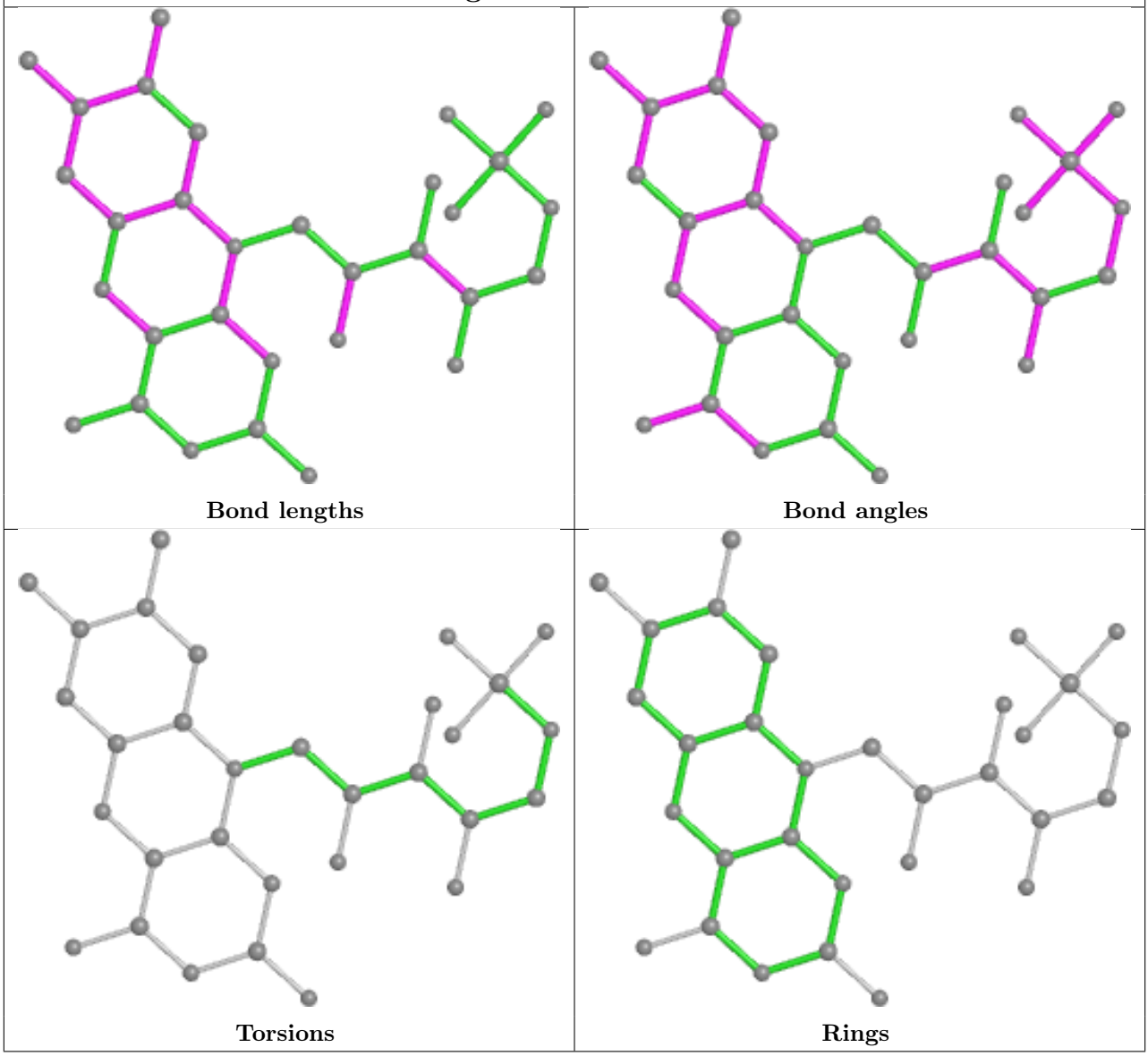


Torsions



Rings

Ligand FMN B 701



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	607/622 (97%)	0.07	17 (2%)	53	54	35, 57, 83, 108	0
1	B	603/622 (96%)	0.19	28 (4%)	32	31	34, 58, 108, 117	0
All	All	1210/1244 (97%)	0.13	45 (3%)	41	41	34, 58, 103, 117	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	LEU	7.0
1	B	64	VAL	5.4
1	B	233	VAL	5.3
1	B	183	ALA	4.5
1	B	143	GLY	4.0
1	A	180	HIS	4.0
1	B	156	LEU	3.8
1	B	187	TYR	3.8
1	B	129	ASP	3.6
1	A	408	SER	3.6
1	A	178	TYR	3.5
1	A	234	GLU	3.4
1	A	501	GLY	3.3
1	B	74	LYS	3.3
1	B	168	PHE	3.3
1	A	235	ALA	3.3
1	B	161	VAL	3.2
1	A	356	ASN	3.1
1	B	190	GLN	3.1
1	B	144	ASP	3.0
1	B	180	HIS	3.0
1	B	158	GLU	2.9
1	B	76	THR	2.9
1	B	230	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	179	GLU	2.8
1	B	153	TYR	2.7
1	A	410	GLY	2.7
1	A	532	GLY	2.6
1	B	231	PHE	2.6
1	A	251	GLU	2.5
1	B	162	ASP	2.5
1	A	233	VAL	2.4
1	B	414	GLU	2.4
1	A	506	ARG	2.3
1	B	152	PHE	2.2
1	B	141	GLY	2.2
1	B	191	ARG	2.2
1	A	570	ASP	2.2
1	B	75	LYS	2.2
1	A	103	HIS	2.2
1	A	252	ASP	2.2
1	B	178	TYR	2.1
1	A	538	ALA	2.1
1	B	184	MET	2.0
1	A	500	ALA	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	A	637	18/19	0.74	0.48	69,109,113,114	0
1	R1A	B	177	18/19	0.75	0.34	103,121,123,123	0
1	R1A	B	637	18/19	0.75	0.37	63,94,98,99	0
1	R1A	A	177	18/19	0.77	0.46	104,130,132,133	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

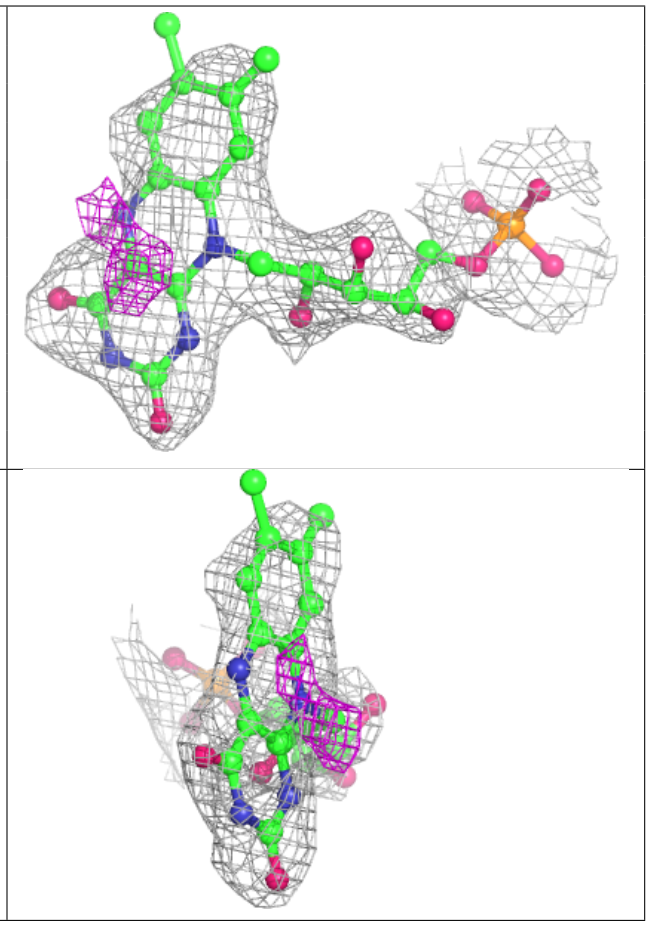
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	B	701	31/31	0.82	0.24	86,91,93,95	0
2	FMN	A	701	31/31	0.92	0.18	69,84,86,86	0
3	FAD	B	702	53/53	0.94	0.18	24,37,45,46	0
4	NAP	B	703	48/48	0.94	0.20	36,45,110,112	0
4	NAP	A	703	48/48	0.96	0.19	33,50,101,102	0
3	FAD	A	702	53/53	0.96	0.19	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.

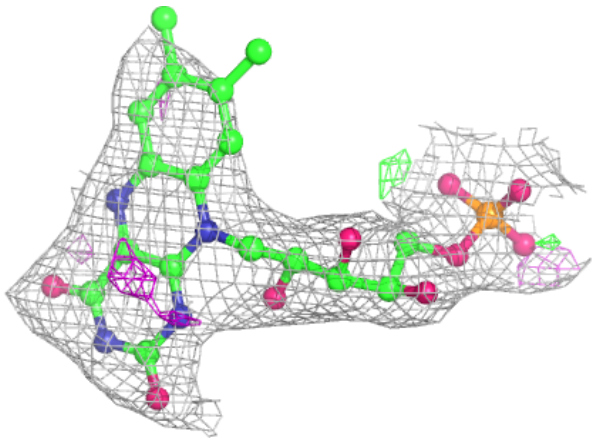
Electron density around FMN B 701:

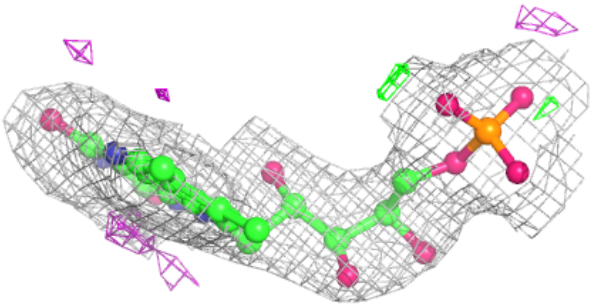
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

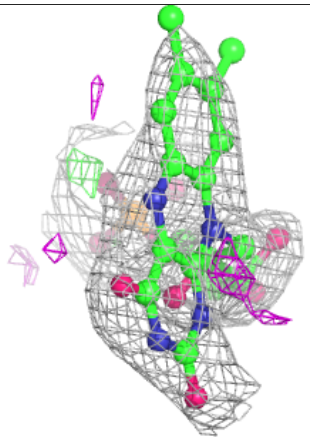


Electron density around FMN A 701:

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

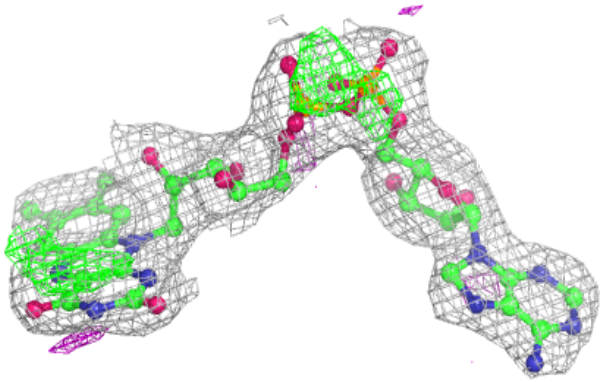


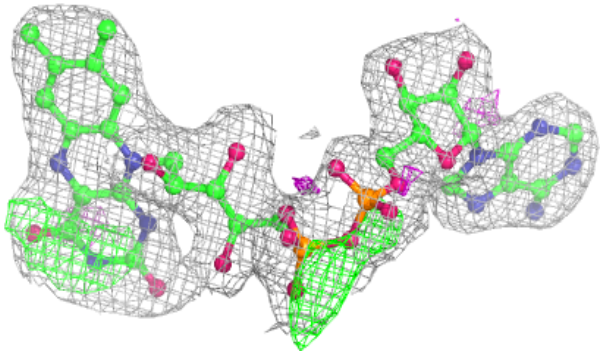


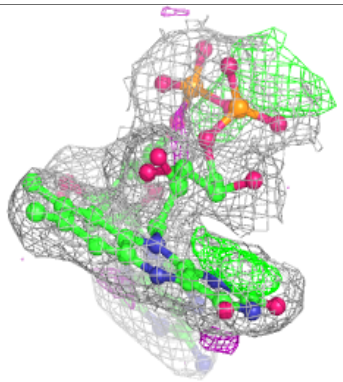


Electron density around FAD B 702:

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

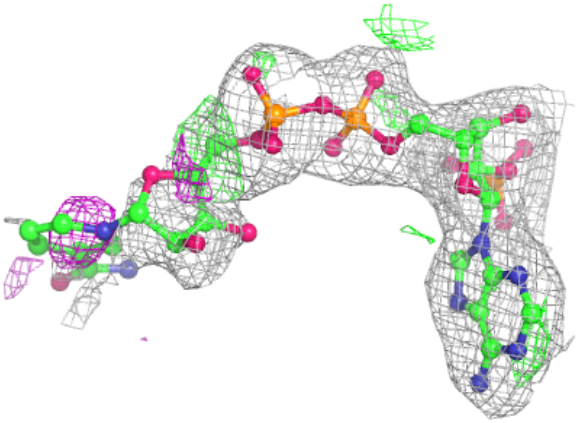


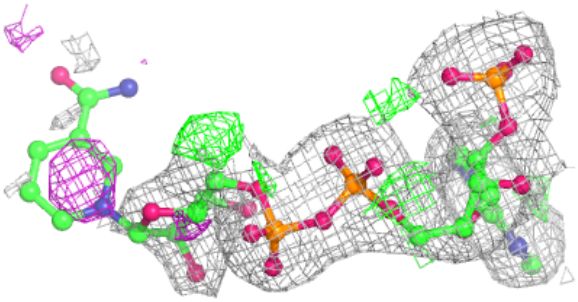


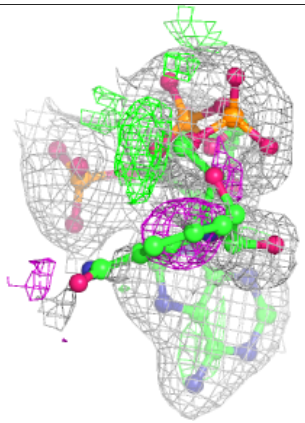


Electron density around NAP B 703:

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

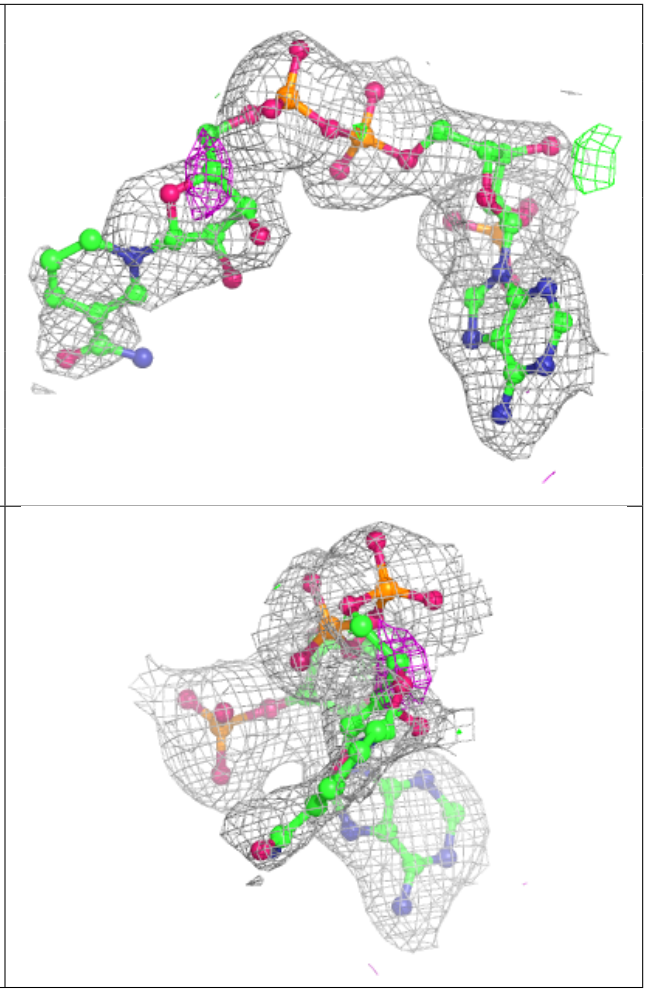






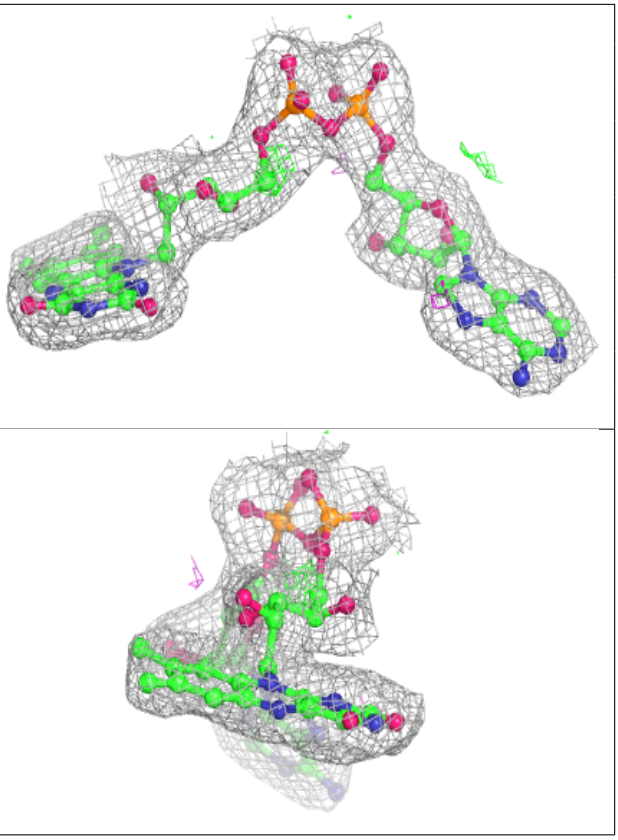
Electron density around NAP A 703:

$2mF_o$-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.