



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:57 PM UTC

PDB ID : 1JA0 / pdb_00001ja0
Title : CYPOR-W677X
Authors : Hubbard, P.A.; Shen, A.L.; Paschke, R.; Kasper, C.B.; Kim, J.J.
Deposited on : 2001-05-29
Resolution : 2.60 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

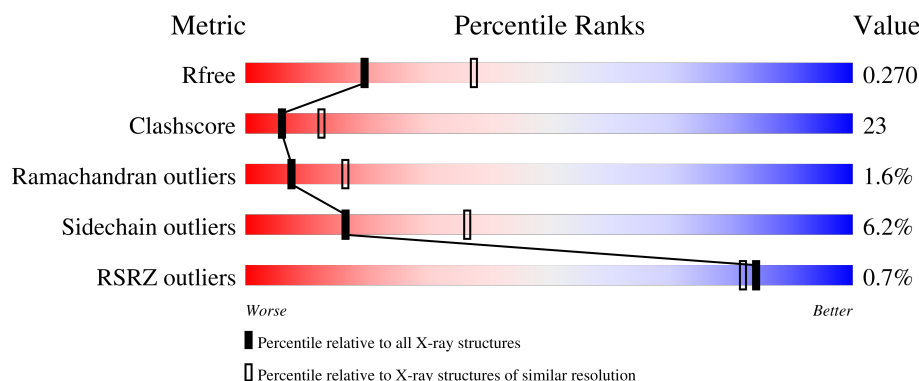
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

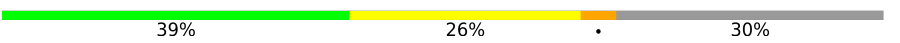
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	620	 55% 38% 5% •
1	B	620	 39% 26% • 30%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8825 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	607	Total	C	N	O	S	12	0	0
			4867	3081	835	928	23			
1	B	432	Total	C	N	O	S	6	0	0
			3468	2196	613	643	16			

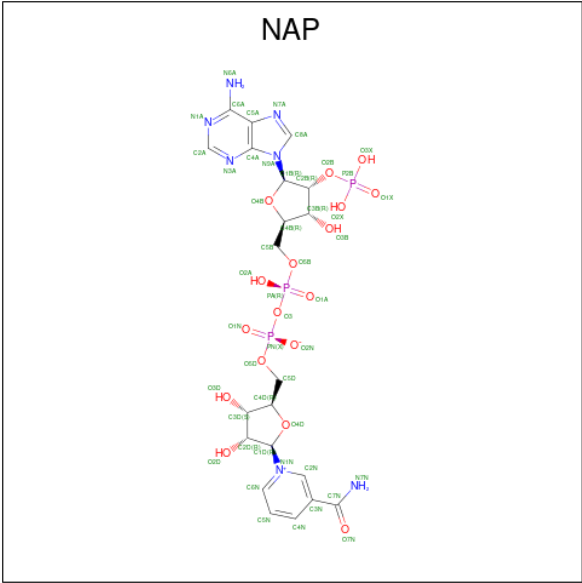
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





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

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total 139	O 139	0	0
5	B	118	Total 118	O 118	0	0

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.

Chain A: 55% 38% 5%

The visualization displays a hierarchical tree structure of 1000 nodes, labeled A1 through Z1000. The nodes are organized into a binary-like hierarchy, with each letter representing a group of 100 nodes. The tree is visualized using a color gradient bar chart, where the color represents a value for each node. The bar chart is positioned above the tree, with the total length representing 1000 nodes. The color gradient indicates a value for each node, with red being the highest (55%), blue being the lowest (38%), and green being in the middle (5%).

The tree structure is as follows:

- A1 to A1000 (1000 nodes)
- B1 to B1000 (1000 nodes)
- C1 to C1000 (1000 nodes)
- D1 to D1000 (1000 nodes)
- E1 to E1000 (1000 nodes)
- F1 to F1000 (1000 nodes)
- G1 to G1000 (1000 nodes)
- H1 to H1000 (1000 nodes)
- I1 to I1000 (1000 nodes)
- J1 to J1000 (1000 nodes)
- K1 to K1000 (1000 nodes)
- L1 to L1000 (1000 nodes)
- M1 to M1000 (1000 nodes)
- N1 to N1000 (1000 nodes)
- O1 to O1000 (1000 nodes)
- P1 to P1000 (1000 nodes)
- Q1 to Q1000 (1000 nodes)
- R1 to R1000 (1000 nodes)
- S1 to S1000 (1000 nodes)
- T1 to T1000 (1000 nodes)
- U1 to U1000 (1000 nodes)
- V1 to V1000 (1000 nodes)
- W1 to W1000 (1000 nodes)
- X1 to X1000 (1000 nodes)
- Y1 to Y1000 (1000 nodes)
- Z1 to Z1000 (1000 nodes)

The bar chart shows the distribution of values across the 1000 nodes. The color gradient indicates a value for each node, with red being the highest (55%), blue being the lowest (38%), and green being in the middle (5%).

Chain B: 39% 26% 30%

ILE GLN THR ALA PRO PRO VAL LYS GLU SER SER PHE VAL GLU LYS MET LYS LYS THR GLY MET ARG ASN ILE ILE PHE VAL TYR GLY SER SER GLN THR GLY GLN THR ALA GLU GLU PHE ASP TRP ALA LEU ASN ARG LEU SER LYS ASP ALA HIS ARG TYR MET LYS MET ARG GLY MET SER ALA ASP PRO GLU TYR ASP LEU ASP LEU SER SER LEU GLU ILE ASP VAL SER LYS LEU VAL VAL PHE CYS MET ALA THR THR TYR GLY GLU GLY ASP PRO THR ASP ASN ALA GLN ASP PHE TYR ASP TRP LEU GLN GLU THR ASP VAL ASP LEU GLY VAL LYS PHE ALA VAL PHE GLY ASP ASN

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.95Å 115.53Å 116.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.1 (30.00-2.60) 82.0 (30.00-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.271 0.209 , 0.270	Depositor DCC
R_{free} test set	1750 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8825	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/4982	1.00	18/6740 (0.3%)
1	B	0.47	0/3550	0.99	17/4805 (0.4%)
All	All	0.47	0/8532	1.00	35/11545 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	ALA	N-CA-C	13.38	129.47	112.89
1	B	354	GLU	N-CA-C	-10.63	92.86	109.76
1	A	69	PHE	CA-C-N	-9.37	108.56	120.56
1	A	69	PHE	C-N-CA	-9.37	108.56	120.56
1	A	406	ALA	N-CA-C	-7.84	103.71	113.28
1	B	297	GLU	N-CA-C	-7.82	102.70	111.07
1	B	548	ALA	N-CA-C	-7.58	103.09	111.36
1	B	413	LYS	N-CA-C	-6.89	104.84	113.18
1	B	666	LEU	N-CA-C	-6.47	103.45	112.45
1	B	645	TYR	N-CA-C	-6.42	104.21	111.14
1	B	511	MET	N-CA-C	6.35	117.50	108.74
1	A	407	SER	N-CA-C	6.34	119.68	110.42
1	B	541	MET	N-CA-C	-6.18	104.09	111.69
1	A	659	ALA	N-CA-C	-6.13	104.15	111.69
1	A	587	ALA	N-CA-C	-6.07	104.78	111.82
1	A	652	GLY	CA-C-N	6.00	127.34	119.84
1	A	652	GLY	C-N-CA	6.00	127.34	119.84
1	A	160	ASP	N-CA-C	-5.96	105.58	114.64
1	A	159	THR	N-CA-C	5.80	117.78	110.24
1	A	548	ALA	N-CA-C	-5.77	105.07	111.71
1	B	596	SER	N-CA-C	5.71	117.50	111.28
1	B	353	GLU	N-CA-C	-5.68	105.18	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	GLY	N-CA-C	-5.63	100.85	112.34
1	B	403	HIS	N-CA-C	-5.41	104.93	112.45
1	B	553	GLN	N-CA-C	-5.38	106.49	112.57
1	A	478	TYR	N-CA-C	5.37	116.44	108.60
1	A	227	VAL	N-CA-C	-5.34	105.12	110.30
1	B	492	SER	N-CA-C	-5.28	105.61	111.36
1	A	301	MET	N-CA-C	5.16	117.52	109.52
1	B	421	VAL	N-CA-C	5.14	115.36	110.53
1	B	532	GLY	CA-C-N	5.11	125.01	119.85
1	B	532	GLY	C-N-CA	5.11	125.01	119.85
1	A	557	VAL	N-CA-C	5.10	115.31	108.17
1	B	620	ILE	N-CA-C	5.10	115.76	110.82
1	A	336	GLU	N-CA-C	5.05	116.86	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4867	0	4716	233	0
1	B	3468	0	3419	150	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
3	A	31	0	19	1	0
4	A	48	0	25	2	0
4	B	48	0	25	2	0
5	A	139	0	0	13	0
5	B	118	0	0	5	0
All	All	8825	0	8266	383	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 23.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ALA:HB2	1:B:676:VAL:HB	1.45	0.97
1:A:338:LEU:HD11	1:A:439:PRO:HD2	1.49	0.94
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.51	0.93
1:A:315:GLU:HB2	1:A:519:ARG:NH1	1.83	0.93
1:A:561:LEU:HD22	1:A:590:GLN:HB2	1.53	0.90
1:B:291:LYS:NZ	5:B:963:HOH:O	2.00	0.90
1:A:480:ALA:O	1:A:481:LYS:HB2	1.74	0.87
1:B:350:ASN:HD22	1:B:351:LEU:N	1.74	0.86
1:B:350:ASN:HD22	1:B:351:LEU:H	1.25	0.85
1:A:315:GLU:HB2	1:A:519:ARG:HH12	1.40	0.84
1:B:400:GLU:OE1	1:B:404:LYS:HE3	1.77	0.84
1:A:388:GLU:OE2	5:A:878:HOH:O	1.96	0.83
1:A:604:TYR:H	1:A:607:HIS:CD2	1.97	0.82
1:A:413:LYS:O	1:A:417:LEU:HG	1.83	0.79
1:A:69:PHE:HD1	1:A:73:MET:HE2	1.48	0.78
1:B:567:ARG:HD3	1:B:597:ARG:NE	1.99	0.78
1:B:437:LEU:O	1:B:438:ARG:HD3	1.84	0.77
1:A:614:GLU:HA	1:A:651:PHE:CE2	2.18	0.77
1:A:465:HIS:ND1	5:A:883:HOH:O	2.16	0.77
1:A:614:GLU:HB3	5:A:881:HOH:O	1.85	0.77
1:A:145:PRO:HB3	1:A:184:MET:SD	2.26	0.75
1:B:479:GLU:HG2	1:B:485:VAL:HG22	1.70	0.73
1:B:620:ILE:HD11	1:B:627:ILE:HD11	1.70	0.73
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.70	0.72
1:A:604:TYR:H	1:A:607:HIS:HD2	1.36	0.72
1:B:266:LEU:HG	1:B:267:LYS:HD3	1.71	0.72
1:A:78:ARG:HD3	1:A:110:MET:HB2	1.71	0.72
1:B:567:ARG:HD3	1:B:597:ARG:CZ	2.19	0.72
1:A:527:PRO:HB2	1:A:625:ALA:CB	2.20	0.72
1:A:318:ASP:OD1	1:A:519:ARG:NH2	2.22	0.71
1:B:354:GLU:O	1:B:355:SER:CB	2.38	0.71
1:A:217:ILE:HD11	1:A:383:THR:HG21	1.74	0.70
1:B:568:ARG:HH11	1:B:568:ARG:HB3	1.57	0.70
1:A:78:ARG:HD2	1:A:110:MET:HE3	1.72	0.69
1:A:450:ARG:HH11	1:A:450:ARG:HB3	1.57	0.69
1:A:651:PHE:O	1:A:652:GLY:C	2.35	0.69
1:A:550:LEU:O	1:A:555:LYS:HB2	1.92	0.69
1:A:548:ALA:O	1:A:552:GLU:HG3	1.94	0.68
1:B:352:ASP:HB3	1:B:354:GLU:O	1.93	0.68
1:A:63:PRO:HG2	1:A:64:VAL:H	1.57	0.67
1:B:613:ARG:HG2	1:B:613:ARG:HH11	1.60	0.67
1:A:423:ALA:O	1:A:482:SER:HB3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LEU:HD13	1:B:543:PHE:CD2	2.30	0.66
1:B:411:GLU:O	1:B:413:LYS:N	2.23	0.66
1:A:576:ARG:HD2	1:A:577:GLU:OE2	1.96	0.65
1:A:302:HIS:HD2	1:A:575:TYR:OH	1.79	0.65
1:A:300:LEU:N	1:A:300:LEU:HD12	2.11	0.65
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.27	0.65
1:B:548:ALA:O	1:B:552:GLU:HG3	1.97	0.65
1:A:76:THR:HG21	1:A:78:ARG:NH1	2.12	0.64
1:A:332:ASN:N	1:A:332:ASN:HD22	1.95	0.64
1:B:297:GLU:HG3	1:B:571:GLU:CD	2.23	0.64
1:A:80:ILE:HG23	1:A:109:GLY:HA2	1.80	0.64
1:B:617:TRP:HZ3	1:B:648:VAL:HG22	1.62	0.64
1:B:567:ARG:HG3	1:B:572:ASP:OD2	1.98	0.64
1:A:87:GLN:HG2	1:A:140:TYR:CE2	2.33	0.63
1:A:292:LEU:HD21	1:A:302:HIS:HB2	1.78	0.63
1:A:78:ARG:CD	1:A:110:MET:HB2	2.27	0.63
1:A:211:ASN:OD1	1:A:214:GLU:HG2	1.98	0.63
1:B:660:VAL:O	1:B:664:LYS:HG2	1.99	0.63
1:A:191:ARG:HH11	1:A:194:GLN:NE2	1.97	0.63
1:A:401:HIS:O	1:A:405:MET:HG3	1.97	0.63
1:B:289:ASN:C	1:B:289:ASN:HD22	2.07	0.63
1:B:425:ARG:HG3	1:B:425:ARG:HH11	1.63	0.63
1:B:624:GLY:HA2	1:B:671:ARG:NH2	2.14	0.63
1:B:354:GLU:O	1:B:355:SER:OG	2.15	0.62
1:A:620:ILE:HD11	1:A:627:ILE:HD11	1.81	0.62
1:A:550:LEU:HD22	1:A:555:LYS:HD3	1.80	0.62
1:B:654:MET:SD	1:B:659:ALA:HA	2.40	0.62
1:B:533:PRO:HD2	1:B:636:MET:HE2	1.81	0.62
1:B:540:PHE:HA	1:B:543:PHE:HB2	1.81	0.62
1:A:657:THR:O	1:A:660:VAL:HG22	1.99	0.61
1:B:620:ILE:CD1	1:B:627:ILE:HD11	2.29	0.61
1:A:245:TYR:HD2	1:A:446:GLU:HG3	1.65	0.61
1:A:390:ALA:O	1:A:399:GLN:HG3	2.00	0.61
1:B:405:MET:HE3	1:B:420:VAL:CG2	2.31	0.61
1:A:450:ARG:HB3	1:A:450:ARG:NH1	2.15	0.61
1:B:568:ARG:HB3	1:B:568:ARG:NH1	2.15	0.61
1:B:411:GLU:C	1:B:413:LYS:H	2.07	0.61
1:A:347:SER:HB3	1:A:363:CYS:HB3	1.82	0.61
1:B:256:ALA:O	1:B:266:LEU:HD21	2.01	0.61
1:B:409:SER:HA	1:B:413:LYS:CD	2.31	0.60
1:B:401:HIS:NE2	1:B:415:LEU:HD21	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:SER:HA	1:B:413:LYS:HD3	1.83	0.60
1:A:76:THR:HG21	1:A:78:ARG:CZ	2.31	0.60
1:A:175:ASN:HD22	1:A:208:ASP:HB3	1.67	0.59
1:B:437:LEU:C	1:B:438:ARG:HD3	2.27	0.59
1:A:125:LEU:HD22	1:A:131:SER:HB2	1.83	0.59
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.84	0.58
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.84	0.58
1:B:259:TYR:CD2	1:B:362:PRO:HB3	2.38	0.58
1:B:676:VAL:C	4:B:852:NAP:N7N	2.62	0.57
1:A:69:PHE:CD1	1:A:73:MET:HE2	2.35	0.57
1:A:346:MET:HE3	1:A:367:TYR:CE1	2.39	0.57
1:A:291:LYS:HE3	5:A:859:HOH:O	2.04	0.57
1:A:336:GLU:CD	1:B:600:ALA:HB2	2.30	0.57
1:B:654:MET:HB2	1:B:658:GLN:HE21	1.69	0.57
1:B:283:LEU:HD22	1:B:510:PRO:HG3	1.87	0.57
1:A:214:GLU:CG	1:A:417:LEU:HD21	2.35	0.57
1:B:648:VAL:HG12	1:B:654:MET:HE3	1.87	0.57
1:B:617:TRP:CZ3	1:B:648:VAL:HG22	2.40	0.56
1:A:427:ILE:HG23	1:A:428:LEU:N	2.20	0.56
1:A:254:ASP:HB2	1:A:257:LYS:HD3	1.87	0.56
1:A:273:LYS:HB2	1:A:273:LYS:NZ	2.20	0.56
1:B:656:HIS:O	1:B:660:VAL:HG13	2.05	0.56
1:B:400:GLU:OE1	1:B:404:LYS:CE	2.50	0.56
1:A:568:ARG:HG2	1:A:598:GLU:HG3	1.87	0.56
1:B:455:TYR:CE2	1:B:514:ARG:HD3	2.40	0.56
1:A:403:HIS:HB3	5:A:866:HOH:O	2.05	0.56
1:A:374:TYR:O	1:A:450:ARG:HD2	2.06	0.55
1:B:297:GLU:HG3	1:B:571:GLU:OE2	2.06	0.55
1:A:350:ASN:HD22	1:A:351:LEU:N	2.04	0.55
1:A:561:LEU:HD23	1:A:589:THR:HB	1.89	0.55
1:A:97:ARG:HA	1:A:100:LYS:HE2	1.87	0.55
1:A:533:PRO:HG2	1:A:636:MET:HG3	1.89	0.55
1:A:314:TYR:O	1:A:462:SER:HB3	2.06	0.55
1:A:156:LEU:HG	1:A:191:ARG:CG	2.37	0.54
1:A:658:GLN:NE2	5:A:872:HOH:O	2.40	0.54
1:A:103:HIS:HA	1:A:107:MET:O	2.07	0.54
1:A:245:TYR:CD2	1:A:446:GLU:HG3	2.41	0.54
1:A:78:ARG:HH11	1:A:110:MET:HE3	1.72	0.54
1:A:417:LEU:O	1:A:422:GLU:HG2	2.07	0.54
1:A:667:MET:HG2	1:A:672:TYR:HB3	1.89	0.54
1:A:253:MET:SD	1:A:364:PRO:HG3	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:HD11	1:B:302:HIS:HB2	1.88	0.54
1:A:175:ASN:OD1	1:A:209:ASP:HB2	2.08	0.54
1:B:250:HIS:HB3	1:B:253:MET:HB2	1.89	0.54
1:A:299:HIS:C	1:A:300:LEU:HD12	2.34	0.53
1:A:428:LEU:O	1:A:432:GLN:HG3	2.09	0.53
1:A:475:ALA:HA	1:A:491:THR:HB	1.91	0.53
1:B:359:HIS:ND1	1:B:363:CYS:HB2	2.23	0.53
1:A:246:GLU:HB2	1:A:351:LEU:CD1	2.39	0.53
1:B:450:ARG:HH11	1:B:450:ARG:HB3	1.74	0.53
1:A:641:GLN:HG3	1:A:672:TYR:OH	2.10	0.52
1:B:652:GLY:O	1:B:653:PRO:C	2.52	0.52
1:A:191:ARG:HH11	1:A:194:GLN:HE21	1.55	0.52
1:A:457:SER:O	1:A:458:ILE:C	2.53	0.52
1:A:285:ALA:HA	1:A:508:LEU:HD23	1.92	0.52
1:A:544:ILE:HD13	1:A:588:LEU:HD11	1.92	0.52
1:B:405:MET:O	5:B:933:HOH:O	2.19	0.52
1:A:384:ASN:HD22	1:A:384:ASN:H	1.58	0.52
1:A:520:LEU:HD13	1:A:543:PHE:CD2	2.44	0.52
1:A:511:MET:O	1:A:512:PHE:HB3	2.10	0.52
1:B:536:GLY:O	1:B:630:CYS:HB3	2.10	0.52
1:B:266:LEU:HG	1:B:267:LYS:CD	2.39	0.51
1:B:541:MET:O	1:B:545:GLN:HG2	2.10	0.51
1:A:73:MET:HE1	1:A:125:LEU:HD21	1.90	0.51
1:A:135:PHE:HB2	1:A:170:VAL:HG22	1.90	0.51
1:A:318:ASP:OD1	1:A:515:LYS:HA	2.11	0.51
1:A:78:ARG:NH1	1:A:110:MET:HE3	2.26	0.51
1:B:540:PHE:O	1:B:544:ILE:HG13	2.10	0.51
1:A:546:GLU:O	1:A:549:TRP:HB3	2.11	0.51
1:A:656:HIS:O	1:A:659:ALA:N	2.27	0.51
1:B:350:ASN:ND2	1:B:351:LEU:N	2.52	0.51
1:A:283:LEU:CD2	1:A:510:PRO:HG3	2.41	0.51
1:A:300:LEU:CD2	1:A:574:LEU:HD21	2.40	0.51
1:B:443:HIS:O	1:B:447:LEU:HG	2.11	0.51
1:A:665:LYS:HG3	1:A:669:LYS:HE3	1.92	0.50
1:A:246:GLU:HB2	1:A:351:LEU:HD13	1.93	0.50
1:A:350:ASN:C	1:A:352:ASP:H	2.18	0.50
1:B:425:ARG:HG3	1:B:425:ARG:NH1	2.26	0.50
1:B:569:SER:HA	1:B:573:TYR:HB2	1.93	0.50
1:A:606:GLN:OE1	4:A:752:NAP:H2A	2.11	0.50
1:A:384:ASN:ND2	1:A:385:VAL:H	2.09	0.50
1:B:352:ASP:O	1:B:354:GLU:O	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:PRO:HG2	1:B:636:MET:HG3	1.92	0.50
1:A:76:THR:HG22	1:A:76:THR:O	2.11	0.50
1:A:214:GLU:CD	1:A:417:LEU:HD21	2.37	0.50
1:A:395:GLU:H	1:A:436:SER:HB2	1.77	0.50
1:A:620:ILE:CD1	1:A:627:ILE:HD11	2.40	0.50
1:A:248:VAL:HG21	1:A:349:ASN:ND2	2.27	0.50
1:B:392:TYR:CD2	1:B:439:PRO:HB3	2.47	0.50
1:A:156:LEU:HG	1:A:191:ARG:HG2	1.93	0.49
1:A:254:ASP:HB2	1:A:257:LYS:CD	2.42	0.49
1:A:465:HIS:CE1	5:A:883:HOH:O	2.60	0.49
1:A:214:GLU:O	1:A:218:THR:HG23	2.12	0.49
1:A:119:LEU:O	1:A:122:LEU:HB2	2.11	0.49
1:A:300:LEU:HD22	1:A:574:LEU:HD21	1.94	0.49
1:B:563:TYR:CZ	1:B:592:ASN:ND2	2.80	0.49
1:A:70:VAL:HG21	1:A:124:SER:HB3	1.94	0.49
1:A:475:ALA:HB1	5:A:823:HOH:O	2.12	0.49
1:B:353:GLU:OE1	1:B:353:GLU:N	2.38	0.49
1:B:563:TYR:CE2	1:B:609:LEU:HD23	2.47	0.49
1:A:87:GLN:HB3	3:A:751:FMN:O2P	2.12	0.49
1:A:208:ASP:HA	1:A:212:LEU:HB2	1.94	0.49
1:A:521:PRO:HB3	1:A:626:HIS:CE1	2.48	0.49
1:A:217:ILE:CD1	1:A:383:THR:HG21	2.41	0.49
1:B:561:LEU:N	1:B:561:LEU:HD12	2.28	0.49
1:B:556:GLU:OE1	5:B:962:HOH:O	2.20	0.49
1:A:625:ALA:N	1:A:671:ARG:HH21	2.11	0.49
1:B:256:ALA:O	1:B:267:LYS:HE2	2.13	0.49
1:B:286:VAL:HG12	1:B:499:PRO:HG3	1.95	0.49
1:A:211:ASN:OD1	1:A:417:LEU:HD22	2.12	0.49
1:A:250:HIS:O	1:A:252:ASP:N	2.46	0.49
1:B:247:LEU:HD12	1:B:248:VAL:H	1.78	0.49
1:A:523:LYS:HG2	5:A:829:HOH:O	2.13	0.48
1:B:594:ALA:HB1	1:B:603:VAL:O	2.13	0.48
1:B:613:ARG:HG2	1:B:613:ARG:NH1	2.29	0.48
1:A:289:ASN:ND2	1:A:303:LEU:HD11	2.28	0.48
1:A:384:ASN:HD22	1:A:384:ASN:N	2.10	0.48
1:B:289:ASN:C	1:B:289:ASN:ND2	2.72	0.48
1:B:667:MET:C	1:B:669:LYS:H	2.21	0.48
1:A:173:LEU:N	1:A:182:ASN:HD21	2.12	0.48
1:B:424:ARG:HD2	5:B:937:HOH:O	2.14	0.48
1:B:405:MET:HE3	1:B:420:VAL:HG23	1.95	0.48
1:B:524:SER:O	1:B:557:VAL:HA	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ILE:HG23	1:A:469:VAL:HG13	1.96	0.48
1:B:398:GLU:OE1	1:B:436:SER:OG	2.26	0.48
1:A:172:GLY:C	1:A:182:ASN:HD21	2.22	0.47
1:B:247:LEU:HG	1:B:248:VAL:N	2.28	0.47
1:A:294:GLN:HE21	1:A:573:TYR:N	2.11	0.47
1:B:352:ASP:O	1:B:355:SER:HB2	2.12	0.47
1:A:140:TYR:HD1	1:A:141:GLY:N	2.12	0.47
1:A:250:HIS:C	1:A:252:ASP:H	2.23	0.47
1:A:337:ILE:HG12	1:A:438:ARG:CZ	2.45	0.47
1:A:388:GLU:O	1:A:391:GLN:HG2	2.15	0.47
1:B:444:LEU:O	1:B:448:LEU:HG	2.15	0.47
1:B:452:GLN:HE21	1:B:452:GLN:HA	1.79	0.47
1:B:606:GLN:OE1	4:B:852:NAP:H2A	2.14	0.47
1:A:427:ILE:HG23	1:A:428:LEU:H	1.80	0.47
1:B:645:TYR:CE1	1:B:660:VAL:HA	2.49	0.47
1:A:276:PHE:HE2	1:A:310:SER:HA	1.79	0.47
1:A:318:ASP:CG	1:A:519:ARG:HH22	2.22	0.47
1:A:665:LYS:CG	1:A:669:LYS:HE3	2.45	0.47
1:B:432:GLN:OE1	1:B:484:ARG:NH2	2.46	0.47
1:A:63:PRO:CG	1:A:64:VAL:H	2.27	0.47
1:A:474:VAL:O	1:A:474:VAL:HG13	2.15	0.47
1:A:537:ILE:HG12	1:A:537:ILE:O	2.14	0.47
1:B:243:ARG:HG3	1:B:244:GLN:H	1.80	0.47
1:A:140:TYR:CD1	1:A:141:GLY:N	2.83	0.46
1:A:544:ILE:CD1	1:A:588:LEU:HD11	2.45	0.46
1:B:498:GLU:HA	1:B:499:PRO:HD3	1.79	0.46
1:A:624:GLY:HA2	1:A:671:ARG:NH2	2.31	0.46
1:B:262:GLU:HA	1:B:269:TYR:CE1	2.51	0.46
1:A:318:ASP:CG	1:A:519:ARG:NH2	2.74	0.46
1:B:566:CYS:HB2	1:B:572:ASP:OD1	2.15	0.46
1:A:253:MET:CG	1:A:254:ASP:N	2.78	0.46
1:A:347:SER:CB	1:A:363:CYS:HB3	2.45	0.46
1:B:408:SER:O	1:B:409:SER:O	2.34	0.46
1:B:537:ILE:HD11	1:B:579:LEU:HD21	1.97	0.46
1:A:329:ALA:O	1:A:333:GLN:HG3	2.16	0.46
1:B:317:GLY:HA3	1:B:518:PHE:O	2.16	0.46
1:B:288:ALA:HB3	1:B:304:GLU:HB2	1.97	0.46
1:B:418:SER:HA	1:B:422:GLU:HB2	1.98	0.46
1:A:64:VAL:HB	5:A:760:HOH:O	2.14	0.46
1:A:535:THR:C	1:A:537:ILE:H	2.23	0.46
1:B:255:VAL:HG23	1:B:256:ALA:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HA	1:A:203:LEU:HD21	1.97	0.45
2:A:750:FAD:H4'	5:A:887:HOH:O	2.16	0.45
1:A:514:ARG:NE	5:A:827:HOH:O	2.49	0.45
1:A:656:HIS:O	1:A:658:GLN:N	2.49	0.45
1:B:530:MET:HE1	1:B:544:ILE:CG1	2.46	0.45
1:A:250:HIS:C	1:A:252:ASP:N	2.74	0.45
1:A:320:VAL:HG12	1:A:456:TYR:O	2.16	0.45
1:B:446:GLU:O	1:B:446:GLU:HG2	2.16	0.45
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.82	0.45
1:B:276:PHE:CD2	1:B:282:PHE:HB2	2.51	0.45
1:B:293:ASN:ND2	1:B:298:ARG:O	2.49	0.45
1:A:70:VAL:HA	1:A:73:MET:HE3	1.97	0.45
1:B:663:VAL:O	1:B:666:LEU:HB2	2.17	0.45
1:A:300:LEU:N	1:A:300:LEU:CD1	2.80	0.45
1:A:530:MET:HE1	1:A:544:ILE:CG1	2.47	0.45
1:A:302:HIS:HE1	1:A:304:GLU:OE2	2.00	0.45
1:A:437:LEU:O	1:A:438:ARG:NH1	2.50	0.45
1:A:346:MET:SD	1:A:346:MET:C	3.00	0.44
1:B:411:GLU:C	1:B:413:LYS:N	2.69	0.44
1:A:334:ILE:O	1:A:338:LEU:HB2	2.17	0.44
1:A:371:LEU:HD23	1:A:375:LEU:HD12	1.98	0.44
1:A:314:TYR:CD1	1:A:314:TYR:C	2.95	0.44
1:B:354:GLU:O	1:B:355:SER:HB2	2.15	0.44
1:B:428:LEU:O	1:B:432:GLN:HG3	2.18	0.44
1:B:519:ARG:HA	1:B:519:ARG:HD3	1.80	0.44
1:A:291:LYS:HE3	1:A:293:ASN:HD21	1.82	0.44
1:B:283:LEU:HB3	1:B:508:LEU:HB3	1.98	0.44
1:A:214:GLU:OE1	1:A:413:LYS:HG3	2.18	0.44
1:A:645:TYR:CD1	1:A:660:VAL:HA	2.53	0.44
1:A:293:ASN:HB3	1:A:300:LEU:HD13	2.00	0.44
1:B:424:ARG:HE	2:B:850:FAD:H1B	1.81	0.44
1:B:570:ASP:C	1:B:570:ASP:OD1	2.61	0.44
1:B:667:MET:CG	1:B:672:TYR:HB3	2.47	0.44
1:A:125:LEU:N	1:A:126:PRO:CD	2.81	0.44
1:A:255:VAL:O	1:A:255:VAL:HG22	2.16	0.44
1:B:525:THR:HG22	1:B:556:GLU:HB3	2.00	0.44
1:A:533:PRO:HD2	1:A:636:MET:HE2	2.00	0.44
1:A:80:ILE:O	1:A:109:GLY:HA2	2.18	0.43
1:A:80:ILE:HD12	1:A:132:LEU:HD23	1.99	0.43
1:A:190:GLN:O	1:A:194:GLN:HG3	2.18	0.43
1:B:318:ASP:OD1	1:B:519:ARG:NH2	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLN:OE1	1:B:428:LEU:HD21	2.18	0.43
1:B:377:ILE:O	1:B:427:ILE:HG22	2.18	0.43
1:B:410:GLY:O	1:B:413:LYS:HB3	2.18	0.43
1:A:88:THR:HG22	1:A:452:GLN:HG3	2.00	0.43
1:A:247:LEU:HD22	1:A:442:ASP:HB3	1.99	0.43
1:A:526:THR:HG23	1:A:624:GLY:O	2.17	0.43
1:B:602:LYS:HG2	1:B:604:TYR:CZ	2.53	0.43
1:B:617:TRP:CZ3	1:B:648:VAL:HG13	2.53	0.43
1:B:638:LYS:HB2	1:B:638:LYS:HE3	1.83	0.43
1:A:338:LEU:CD1	1:A:439:PRO:HD2	2.33	0.43
1:A:518:PHE:CD1	1:A:675:ASP:HB2	2.53	0.43
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.99	0.43
1:A:416:TYR:HD2	1:A:417:LEU:HD23	1.83	0.43
1:A:530:MET:HE1	1:A:544:ILE:HG12	1.99	0.43
1:B:380:PRO:HA	1:B:381:PRO:HD3	1.94	0.43
1:B:575:TYR:O	1:B:578:GLU:HG2	2.18	0.43
1:B:561:LEU:HG	1:B:590:GLN:HB2	2.01	0.43
1:A:304:GLU:HG2	1:A:470:HIS:CD2	2.54	0.43
1:A:538:ALA:HB3	1:A:539:PRO:CD	2.48	0.43
1:B:403:HIS:C	1:B:405:MET:H	2.26	0.43
1:A:180:HIS:HB3	1:A:183:ALA:HB2	2.00	0.43
1:A:342:LEU:HA	1:A:367:TYR:HB2	2.00	0.43
1:A:175:ASN:ND2	1:A:208:ASP:HB3	2.34	0.42
1:B:385:VAL:HG23	1:B:447:LEU:HB3	1.99	0.42
1:A:294:GLN:HE21	1:A:573:TYR:H	1.66	0.42
1:A:283:LEU:HD22	1:A:510:PRO:HG3	2.00	0.42
1:A:676:VAL:C	4:A:752:NAP:N7N	2.77	0.42
1:B:651:PHE:N	1:B:651:PHE:CD1	2.87	0.42
1:A:88:THR:HG22	1:A:88:THR:O	2.20	0.42
1:A:191:ARG:NH1	1:A:194:GLN:HE21	2.16	0.42
1:B:404:LYS:HA	1:B:407:SER:OG	2.20	0.42
1:A:82:VAL:HG13	1:A:134:VAL:HB	2.00	0.42
1:A:294:GLN:NE2	1:A:573:TYR:O	2.52	0.42
1:A:332:ASN:N	1:A:332:ASN:ND2	2.66	0.42
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.84	0.42
1:A:451:LEU:HD11	1:A:489:VAL:HG11	2.01	0.42
1:A:549:TRP:O	1:A:553:GLN:HB2	2.19	0.42
1:A:657:THR:HB	5:A:843:HOH:O	2.19	0.42
1:A:240:SER:O	1:A:241:SER:CB	2.68	0.42
1:A:350:ASN:C	1:A:352:ASP:N	2.77	0.42
1:A:493:TRP:HH2	1:A:510:PRO:HD2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLU:HA	1:A:651:PHE:CZ	2.54	0.42
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.84	0.42
1:A:380:PRO:HA	1:A:381:PRO:HD3	1.93	0.42
1:A:606:GLN:HE21	1:A:639:ASP:HB3	1.85	0.42
1:A:272:GLN:OE1	1:A:282:PHE:HA	2.20	0.42
1:A:276:PHE:CG	1:A:282:PHE:HB2	2.54	0.42
1:B:612:ASP:C	1:B:614:GLU:N	2.78	0.42
1:A:472:CYS:HB2	1:A:575:TYR:OH	2.20	0.41
1:B:330:LEU:HD12	1:B:330:LEU:HA	1.89	0.41
1:A:80:ILE:HG23	1:A:109:GLY:CA	2.50	0.41
1:A:297:GLU:HG3	1:A:571:GLU:CD	2.45	0.41
1:B:468:SER:HB2	5:B:912:HOH:O	2.20	0.41
1:A:79:ASN:O	1:A:131:SER:HA	2.20	0.41
1:A:248:VAL:HG21	1:A:349:ASN:HD21	1.85	0.41
1:A:349:ASN:HA	1:A:358:LYS:O	2.21	0.41
1:B:409:SER:HA	1:B:413:LYS:HD2	2.00	0.41
1:B:608:LEU:O	1:B:611:ARG:HB3	2.19	0.41
1:A:135:PHE:CE2	1:A:192:LEU:HD11	2.56	0.41
1:A:294:GLN:HG2	1:A:571:GLU:C	2.46	0.41
1:B:314:TYR:CE2	1:B:458:ILE:HG21	2.56	0.41
1:A:120:ALA:C	1:A:122:LEU:H	2.28	0.41
1:B:401:HIS:CD2	1:B:415:LEU:HD21	2.56	0.41
1:A:346:MET:HE1	1:A:348:LEU:HG	2.02	0.41
1:A:651:PHE:N	1:A:651:PHE:CD1	2.89	0.41
1:A:78:ARG:HD3	1:A:109:GLY:O	2.21	0.41
1:A:555:LYS:HB3	1:A:555:LYS:HE2	1.90	0.41
1:B:488:GLY:HA3	2:B:850:FAD:O2P	2.21	0.41
1:B:530:MET:HE1	1:B:544:ILE:HG12	2.02	0.41
1:B:568:ARG:HH11	1:B:568:ARG:CB	2.30	0.41
1:B:633:ALA:HB2	1:B:676:VAL:CB	2.32	0.41
1:A:98:LEU:O	1:A:101:ASP:HB2	2.21	0.41
1:A:356:ASN:HD22	1:A:356:ASN:HA	1.69	0.41
1:A:535:THR:C	1:A:537:ILE:N	2.78	0.41
1:A:561:LEU:CD2	1:A:589:THR:HB	2.50	0.41
1:A:564:TYR:CG	1:A:565:GLY:N	2.89	0.41
1:B:520:LEU:HD13	1:B:543:PHE:CG	2.56	0.41
1:B:617:TRP:CZ2	1:B:621:HIS:CG	3.09	0.41
1:B:652:GLY:O	1:B:654:MET:HG2	2.20	0.41
1:A:590:GLN:HB3	1:A:592:ASN:OD1	2.21	0.41
1:B:395:GLU:HA	1:B:396:PRO:HD2	1.90	0.41
1:B:405:MET:HG3	1:B:416:TYR:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:SER:O	1:A:409:SER:CB	2.69	0.40
1:B:274:PRO:HB3	1:B:276:PHE:CE1	2.55	0.40
1:B:378:THR:O	1:B:426:HIS:HB3	2.21	0.40
1:A:69:PHE:O	1:A:70:VAL:C	2.57	0.40
1:A:384:ASN:ND2	1:A:385:VAL:N	2.69	0.40
1:B:549:TRP:HA	1:B:552:GLU:OE1	2.21	0.40
1:A:253:MET:HG2	1:A:254:ASP:N	2.35	0.40
1:A:419:TRP:O	1:A:425:ARG:NH1	2.53	0.40
1:A:533:PRO:HG2	1:A:636:MET:CG	2.49	0.40
1:B:247:LEU:CG	1:B:248:VAL:N	2.85	0.40
1:B:276:PHE:CG	1:B:282:PHE:HB2	2.57	0.40
1:B:346:MET:SD	1:B:348:LEU:CD2	3.09	0.40
1:B:419:TRP:O	1:B:425:ARG:NH1	2.54	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	603/620 (97%)	533 (88%)	59 (10%)	11 (2%)	6	14
1	B	428/620 (69%)	390 (91%)	32 (8%)	6 (1%)	9	19
All	All	1031/1240 (83%)	923 (90%)	91 (9%)	17 (2%)	7	16

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	SER
1	A	409	SER
1	A	657	THR
1	B	355	SER
1	B	409	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	411	GLU
1	A	238	GLU
1	A	251	GLU
1	A	481	LYS
1	B	412	GLY
1	B	653	PRO
1	A	656	HIS
1	A	68	SER
1	A	233	VAL
1	B	408	SER
1	A	64	VAL
1	A	458	ILE

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	521/529 (98%)	487 (94%)	34 (6%)	15	35
1	B	372/529 (70%)	351 (94%)	21 (6%)	19	40
All	All	893/1058 (84%)	838 (94%)	55 (6%)	16	36

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	93	GLU
1	A	122	LEU
1	A	142	GLU
1	A	151	ASP
1	A	156	LEU
1	A	221	GLU
1	A	234	GLU
1	A	262	GLU
1	A	271	ASN
1	A	273	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	294	GLN
1	A	303	LEU
1	A	332	ASN
1	A	338	LEU
1	A	346	MET
1	A	351	LEU
1	A	354	GLU
1	A	384	ASN
1	A	400	GLU
1	A	424	ARG
1	A	439	PRO
1	A	450	ARG
1	A	481	LYS
1	A	517	GLN
1	A	520	LEU
1	A	553	GLN
1	A	569	SER
1	A	578	GLU
1	A	588	LEU
1	A	616	LEU
1	A	643	THR
1	A	657	THR
1	A	665	LYS
1	B	260	THR
1	B	289	ASN
1	B	294	GLN
1	B	313	ARG
1	B	338	LEU
1	B	356	ASN
1	B	371	LEU
1	B	375	LEU
1	B	385	VAL
1	B	400	GLU
1	B	405	MET
1	B	407	SER
1	B	422	GLU
1	B	442	ASP
1	B	450	ARG
1	B	452	GLN
1	B	484	ARG
1	B	578	GLU
1	B	579	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	616	LEU
1	B	657	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	182	ASN
1	A	194	GLN
1	A	294	GLN
1	A	299	HIS
1	A	302	HIS
1	A	319	HIS
1	A	326	ASN
1	A	332	ASN
1	A	349	ASN
1	A	350	ASN
1	A	356	ASN
1	A	384	ASN
1	A	391	GLN
1	A	452	GLN
1	A	517	GLN
1	A	553	GLN
1	A	590	GLN
1	A	607	HIS
1	A	642	ASN
1	B	280	ASN
1	B	289	ASN
1	B	332	ASN
1	B	349	ASN
1	B	350	ASN
1	B	356	ASN
1	B	384	ASN
1	B	391	GLN
1	B	399	GLN
1	B	452	GLN
1	B	470	HIS
1	B	486	ASN
1	B	517	GLN
1	B	545	GLN
1	B	583	HIS
1	B	590	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	592	ASN
1	B	599	GLN
1	B	635	ASN
1	B	642	ASN
1	B	658	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	FAD	A	750	-	58,58,58	2.28	22 (37%)	85,89,89	1.34	12 (14%)
4	NAP	B	852	-	50,52,52	3.67	17 (34%)	71,80,80	1.35	10 (14%)
3	FMN	A	751	-	33,33,33	1.87	12 (36%)	48,50,50	1.67	10 (20%)
4	NAP	A	752	-	50,52,52	3.61	19 (38%)	71,80,80	1.37	8 (11%)
2	FAD	B	850	-	58,58,58	2.55	22 (37%)	85,89,89	1.35	12 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	750	-	-	3/34/50/50	0/6/6/6
4	NAP	B	852	-	-	6/35/67/67	0/5/5/5
3	FMN	A	751	-	-	3/18/18/18	0/3/3/3
4	NAP	A	752	-	-	9/35/67/67	0/5/5/5
2	FAD	B	850	-	-	1/34/50/50	0/6/6/6

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	752	NAP	C2N-N1N	14.66	1.51	1.35
4	B	852	NAP	C2N-N1N	13.73	1.50	1.35
4	B	852	NAP	C4N-C3N	11.14	1.56	1.39
4	A	752	NAP	C4N-C3N	10.26	1.55	1.39
4	A	752	NAP	C4A-N3A	7.38	1.48	1.34
4	B	852	NAP	C4A-N3A	7.22	1.47	1.34
4	B	852	NAP	C7N-N7N	6.74	1.45	1.33
2	B	850	FAD	C10-N10	6.64	1.51	1.37
2	B	850	FAD	P-O3P	-6.39	1.52	1.59
4	B	852	NAP	C6N-C5N	6.26	1.51	1.38
4	B	852	NAP	PN-O3	-6.15	1.52	1.59
4	A	752	NAP	C6N-C5N	6.09	1.51	1.38
4	A	752	NAP	C7N-N7N	5.87	1.43	1.33
4	B	852	NAP	PA-O3	-5.83	1.53	1.59
2	B	850	FAD	C5'-C4'	-5.82	1.43	1.51
4	A	752	NAP	PA-O3	-5.55	1.53	1.59
2	A	750	FAD	C10-N10	5.53	1.49	1.37
2	B	850	FAD	PA-O3P	-5.41	1.53	1.59
2	A	750	FAD	C2'-C3'	5.15	1.62	1.53
4	B	852	NAP	P2B-O2B	-4.93	1.50	1.59
4	A	752	NAP	PN-O3	-4.88	1.54	1.59
4	B	852	NAP	C5A-C6A	4.72	1.54	1.41
2	B	850	FAD	C2'-C3'	4.62	1.61	1.53
2	A	750	FAD	C5'-C4'	-4.60	1.45	1.51
2	A	750	FAD	P-O3P	-4.54	1.54	1.59
4	A	752	NAP	C5A-C6A	4.53	1.53	1.41
4	A	752	NAP	P2B-O2B	-4.50	1.51	1.59
2	B	850	FAD	C1'-C2'	4.44	1.58	1.52
4	B	852	NAP	C2A-N1A	4.43	1.41	1.33
2	B	850	FAD	C4A-N3A	4.32	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	752	NAP	C2A-N1A	4.27	1.41	1.33
2	A	750	FAD	C4X-N5	4.17	1.39	1.30
2	A	750	FAD	C4A-N3A	4.01	1.41	1.34
2	B	850	FAD	C4X-N5	3.84	1.39	1.30
3	A	751	FMN	C9A-C5A	3.83	1.47	1.41
2	A	750	FAD	C8A-N7A	3.83	1.39	1.31
2	B	850	FAD	C8A-N7A	3.73	1.38	1.31
2	A	750	FAD	C9A-C5X	3.70	1.47	1.41
2	B	850	FAD	C6-C5X	3.56	1.45	1.40
2	A	750	FAD	C6-C5X	3.51	1.45	1.40
2	A	750	FAD	C9A-N10	3.50	1.47	1.41
2	A	750	FAD	PA-O3P	-3.50	1.55	1.59
2	B	850	FAD	C9A-N10	3.47	1.47	1.41
3	A	751	FMN	C10-N10	3.24	1.44	1.37
4	A	752	NAP	C5D-C4D	3.23	1.61	1.51
3	A	751	FMN	C4A-N5	3.15	1.37	1.30
2	A	750	FAD	C1'-C2'	3.12	1.57	1.52
2	B	850	FAD	C9A-C5X	3.11	1.46	1.41
2	A	750	FAD	PA-O5B	-2.97	1.47	1.59
3	A	751	FMN	C9A-N10	2.93	1.46	1.41
4	B	852	NAP	PN-O5D	-2.90	1.48	1.59
2	B	850	FAD	C5A-C4A	2.90	1.44	1.39
3	A	751	FMN	C8-C7	2.90	1.47	1.40
3	A	751	FMN	P-O5'	2.87	1.69	1.60
2	B	850	FAD	C10-N1	2.83	1.38	1.33
4	B	852	NAP	C5D-C4D	2.79	1.59	1.51
2	A	750	FAD	C5A-C4A	2.76	1.44	1.39
3	A	751	FMN	C9-C8	-2.76	1.35	1.39
3	A	751	FMN	C9-C9A	2.72	1.44	1.39
4	B	852	NAP	C5A-N7A	2.70	1.44	1.39
4	A	752	NAP	PA-O5B	-2.65	1.49	1.59
2	B	850	FAD	O2'-C2'	2.64	1.48	1.43
3	A	751	FMN	C8M-C8	2.62	1.55	1.51
2	A	750	FAD	C8-C7	2.61	1.47	1.40
2	A	750	FAD	C10-N1	2.60	1.38	1.33
4	A	752	NAP	C5A-N7A	2.59	1.43	1.39
3	A	751	FMN	O4-C4	2.53	1.28	1.23
2	B	850	FAD	C8-C7	2.52	1.47	1.40
2	A	750	FAD	C9-C9A	2.50	1.43	1.39
4	A	752	NAP	PN-O5D	-2.49	1.49	1.59
2	B	850	FAD	C6-C7	2.49	1.43	1.39
4	A	752	NAP	C4A-N9A	-2.47	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	850	FAD	C9-C9A	2.43	1.43	1.39
2	A	750	FAD	O2'-C2'	2.41	1.48	1.43
2	B	850	FAD	PA-O5B	-2.38	1.50	1.59
4	B	852	NAP	C4A-N9A	-2.36	1.32	1.37
4	B	852	NAP	PA-O5B	-2.31	1.50	1.59
2	B	850	FAD	O2B-C2B	2.27	1.48	1.43
2	B	850	FAD	C5B-C4B	2.25	1.58	1.51
2	A	750	FAD	C6-C7	2.24	1.42	1.39
2	B	850	FAD	C1B-N9A	2.22	1.52	1.46
4	A	752	NAP	P2B-O2X	-2.21	1.46	1.54
3	A	751	FMN	P-O1P	2.20	1.57	1.50
3	A	751	FMN	O2'-C2'	2.16	1.47	1.43
2	A	750	FAD	C7M-C7	2.08	1.54	1.51
2	A	750	FAD	C2A-N1A	2.08	1.37	1.33
4	A	752	NAP	O4D-C1D	2.06	1.43	1.40
4	B	852	NAP	P2B-O2X	-2.06	1.47	1.54
4	B	852	NAP	PA-O2A	-2.04	1.45	1.55
4	A	752	NAP	PA-O2A	-2.03	1.45	1.55
4	A	752	NAP	C5A-C4A	-2.03	1.35	1.39
2	A	750	FAD	C5B-C4B	2.02	1.57	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	751	FMN	C9A-C5A-N5	4.80	127.55	122.45
3	A	751	FMN	C4'-C3'-C2'	-4.22	106.54	113.57
2	A	750	FAD	C4'-C3'-C2'	4.20	120.56	113.57
4	A	752	NAP	C4D-O4D-C1D	3.91	113.51	109.92
2	B	850	FAD	C4'-C3'-C2'	3.76	119.82	113.57
2	B	850	FAD	C9A-C5X-N5	3.73	126.42	122.45
2	A	750	FAD	C9A-C5X-N5	3.53	126.20	122.45
4	A	752	NAP	N6A-C6A-N1A	3.51	126.19	118.38
4	A	752	NAP	O4B-C1B-N9A	3.45	114.72	108.09
4	B	852	NAP	N6A-C6A-N1A	3.44	126.04	118.38
3	A	751	FMN	C5A-N5-C4A	-3.43	112.54	118.09
4	B	852	NAP	O4B-C1B-N9A	3.36	114.54	108.09
3	A	751	FMN	O4'-C4'-C3'	-3.32	101.48	109.25
2	B	850	FAD	C2'-C1'-N10	-3.22	94.98	110.20
4	B	852	NAP	C4D-O4D-C1D	3.21	112.86	109.92
4	A	752	NAP	C2A-N1A-C6A	3.14	123.89	118.73
4	A	752	NAP	N3A-C2A-N1A	-2.95	124.11	128.58
4	B	852	NAP	C2A-N1A-C6A	2.92	123.53	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	850	FAD	C5X-C9A-N10	-2.88	115.36	117.97
2	A	750	FAD	O2-C2-N3	2.85	124.05	118.58
2	A	750	FAD	C5X-C9A-N10	-2.79	115.45	117.97
4	B	852	NAP	N3A-C2A-N1A	-2.77	124.39	128.58
2	B	850	FAD	O5'-C5'-C4'	2.72	116.63	109.36
4	B	852	NAP	O7N-C7N-C3N	2.70	122.90	119.60
2	A	750	FAD	O3'-C3'-C4'	-2.66	102.88	108.93
2	A	750	FAD	C9-C9A-N10	2.63	125.39	121.85
2	A	750	FAD	C2'-C1'-N10	-2.63	97.76	110.20
3	A	751	FMN	C5A-C9A-N10	-2.62	115.60	117.97
2	A	750	FAD	C1B-N9A-C8A	2.59	132.85	127.09
2	B	850	FAD	O2-C2-N3	2.59	123.54	118.58
2	B	850	FAD	C2B-C1B-N9A	2.56	119.67	113.30
2	B	850	FAD	C9-C9A-N10	2.56	125.29	121.85
4	B	852	NAP	C5A-C4A-N3A	-2.55	123.20	126.72
3	A	751	FMN	O4'-C4'-C5'	-2.51	104.45	109.99
4	A	752	NAP	C5A-C4A-N3A	-2.48	123.30	126.72
3	A	751	FMN	O3P-P-O5'	-2.46	100.26	106.67
2	B	850	FAD	C1B-N9A-C8A	2.44	132.51	127.09
2	B	850	FAD	C10-N1-C2	2.39	122.03	116.85
2	A	750	FAD	C10-N1-C2	2.36	121.95	116.85
4	A	752	NAP	O7N-C7N-C3N	2.34	122.46	119.60
3	A	751	FMN	C6-C5A-N5	-2.28	114.67	118.44
2	A	750	FAD	O4B-C1B-N9A	-2.26	103.76	108.09
3	A	751	FMN	C7M-C7-C6	-2.25	115.60	119.57
2	A	750	FAD	C2B-C1B-N9A	2.21	118.79	113.30
4	A	752	NAP	O7N-C7N-N7N	-2.20	119.44	122.62
4	B	852	NAP	O7N-C7N-N7N	-2.15	119.51	122.62
4	B	852	NAP	O2N-PN-O3	2.15	113.08	107.27
2	A	750	FAD	C1'-N10-C9A	2.14	124.79	120.63
2	B	850	FAD	O3'-C3'-C4'	-2.11	104.13	108.93
3	A	751	FMN	O2'-C2'-C3'	2.11	114.19	109.25
2	B	850	FAD	O3B-C3B-C2B	-2.02	105.33	111.82
4	B	852	NAP	C2N-N1N-C1D	-2.02	114.68	119.13

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	852	NAP	C2B-C1B-N9A-C8A
4	B	852	NAP	C2B-C1B-N9A-C4A
4	A	752	NAP	C2B-C1B-N9A-C8A

Continued on next page...

Continued from previous page...

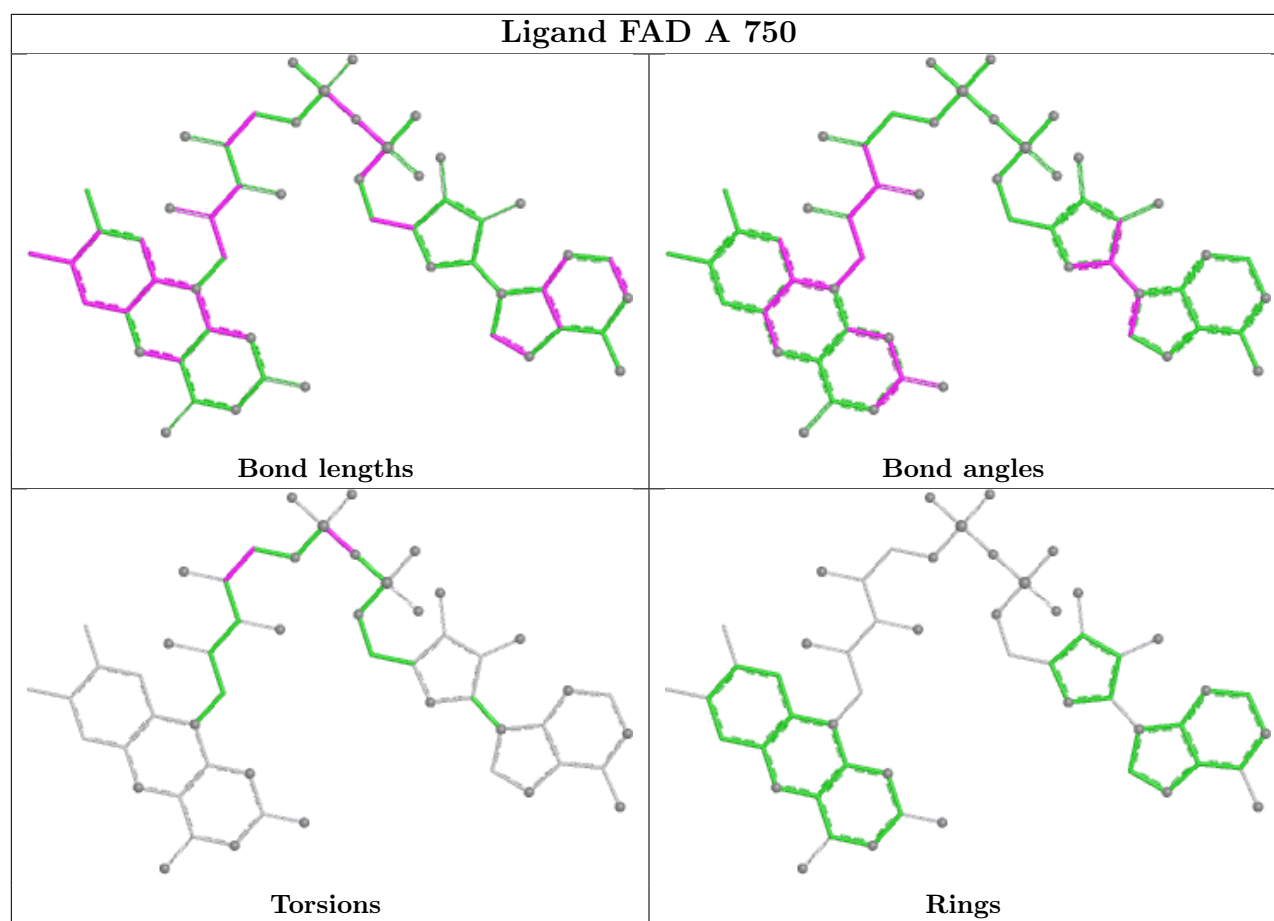
Mol	Chain	Res	Type	Atoms
2	A	750	FAD	C3'-C4'-C5'-O5'
2	A	750	FAD	PA-O3P-P-O1P
2	B	850	FAD	PA-O3P-P-O1P
4	A	752	NAP	PA-O3-PN-O1N
4	B	852	NAP	PA-O3-PN-O1N
4	A	752	NAP	C2B-C1B-N9A-C4A
3	A	751	FMN	O2'-C2'-C3'-O3'
4	A	752	NAP	O4D-C1D-N1N-C2N
4	A	752	NAP	O4D-C1D-N1N-C6N
3	A	751	FMN	C1'-C2'-C3'-O3'
3	A	751	FMN	O2'-C2'-C3'-C4'
4	A	752	NAP	O4B-C1B-N9A-C8A
4	A	752	NAP	O4D-C4D-C5D-O5D
4	B	852	NAP	O4D-C4D-C5D-O5D
4	A	752	NAP	C2B-O2B-P2B-O2X
4	B	852	NAP	C2B-O2B-P2B-O2X
2	A	750	FAD	PA-O3P-P-O2P
4	A	752	NAP	PA-O3-PN-O2N
4	B	852	NAP	PA-O3-PN-O2N

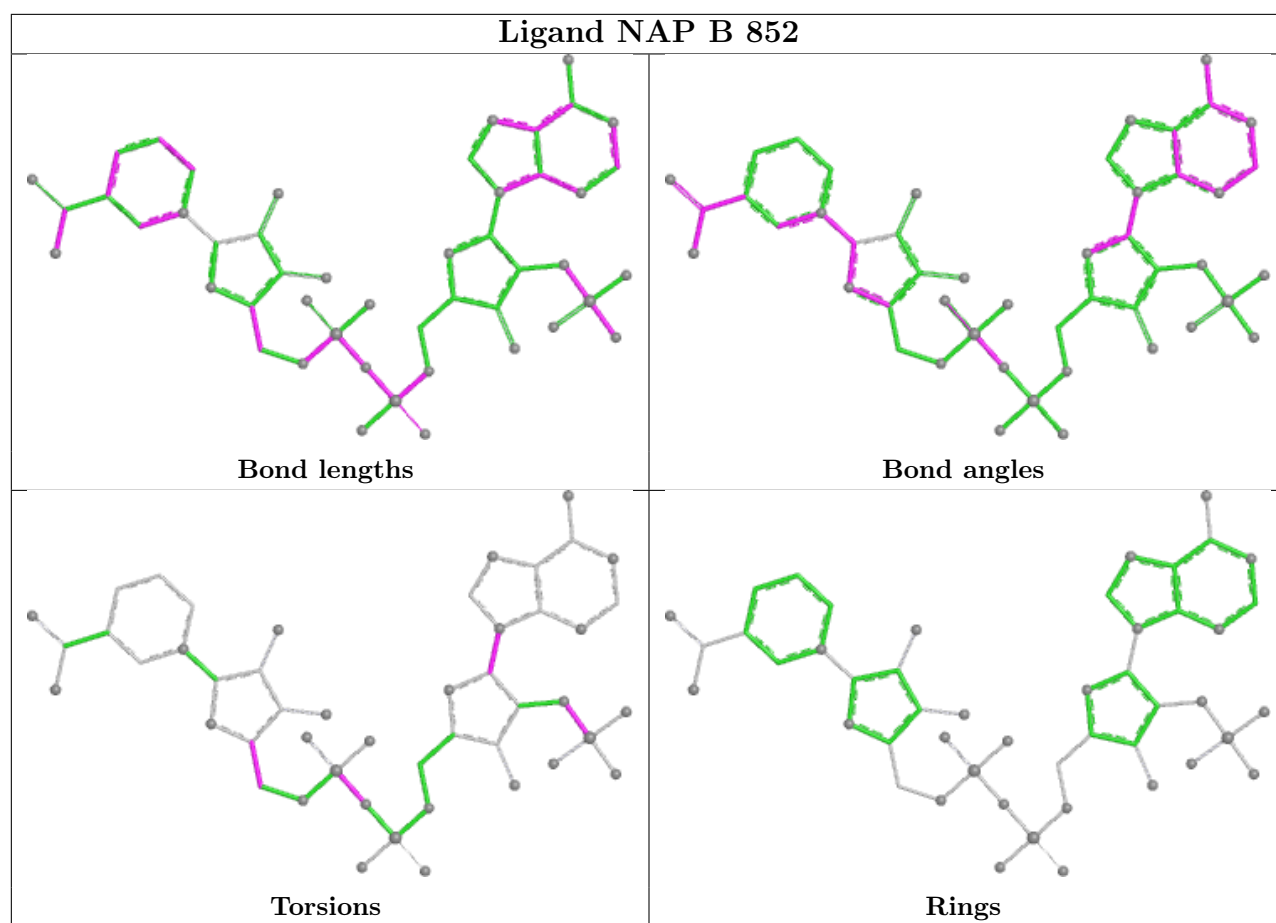
There are no ring outliers.

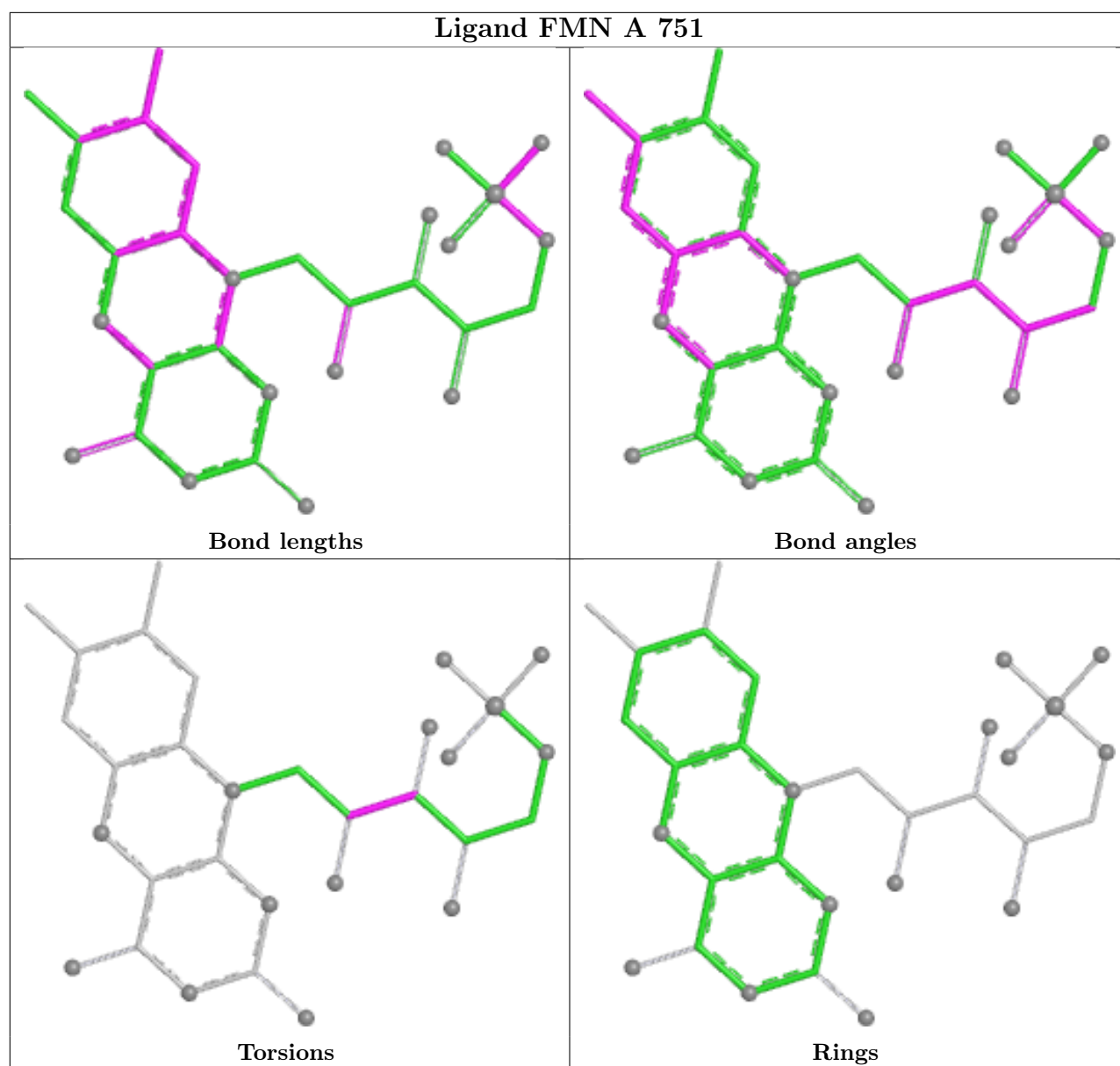
5 monomers are involved in 8 short contacts:

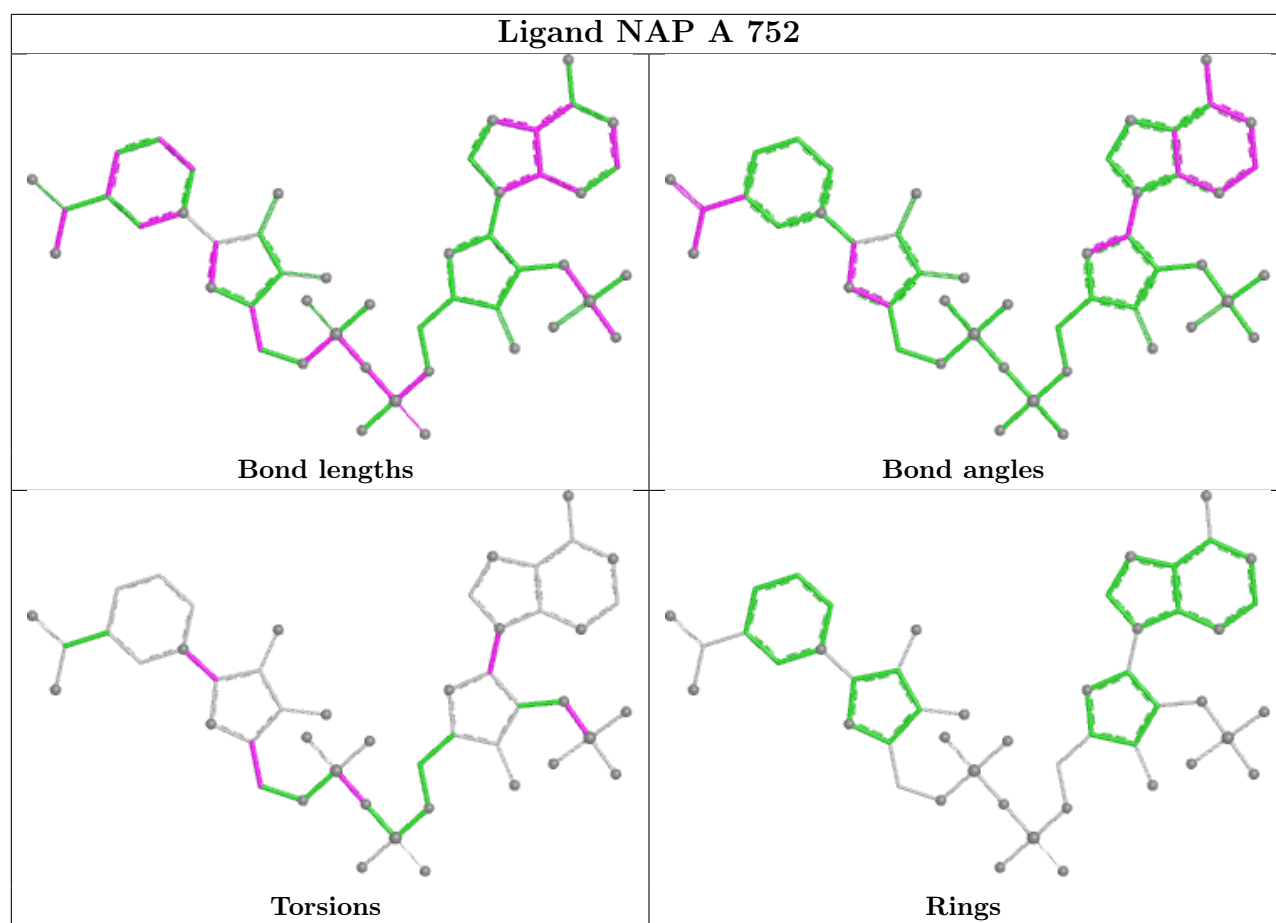
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	FAD	1	0
4	B	852	NAP	2	0
3	A	751	FMN	1	0
4	A	752	NAP	2	0
2	B	850	FAD	2	0

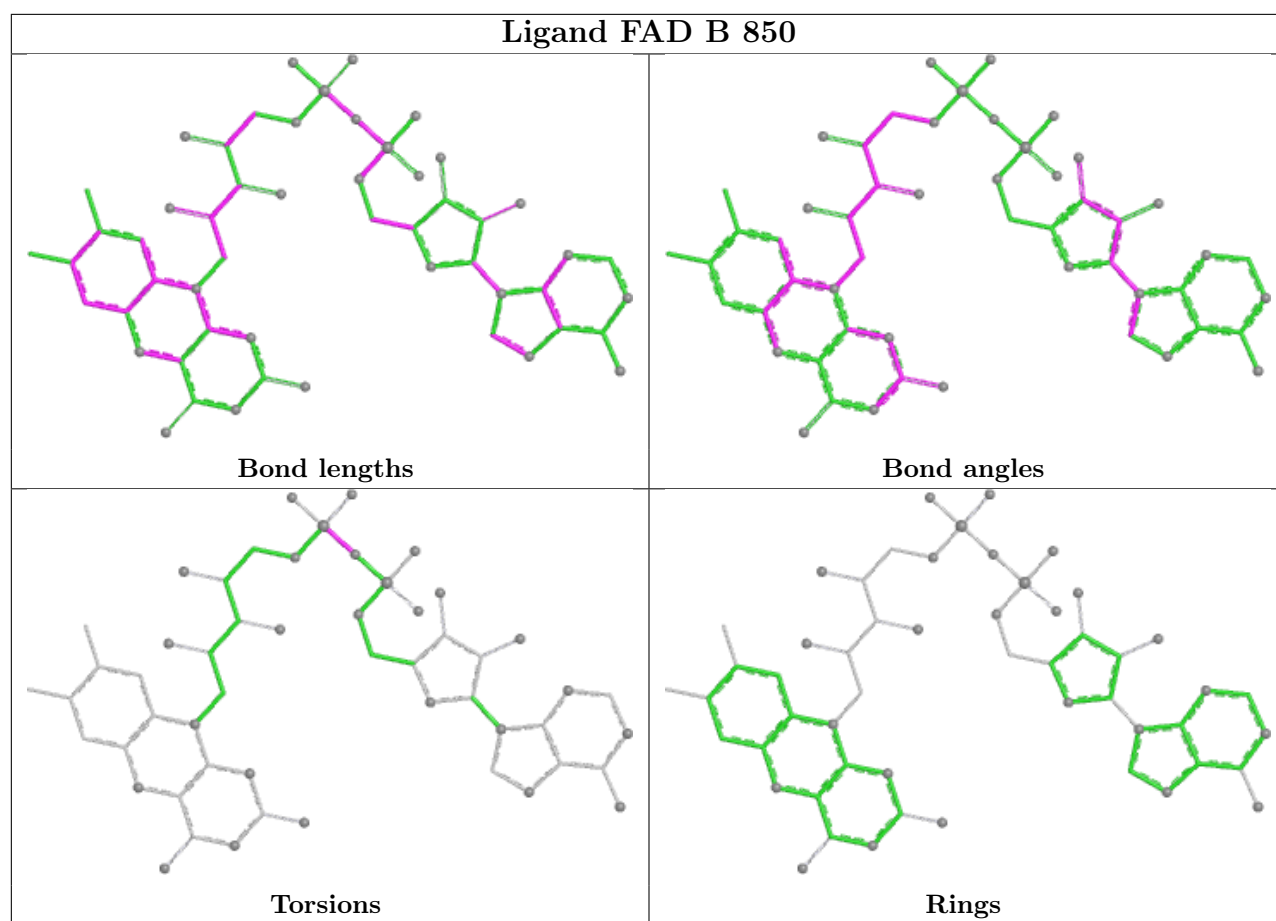
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	607/620 (97%)	-0.32	5 (0%)	82 80	22, 43, 71, 101	11 (1%)
1	B	432/620 (69%)	-0.34	2 (0%)	87 85	19, 41, 80, 98	6 (1%)
All	All	1039/1240 (83%)	-0.33	7 (0%)	84 82	19, 42, 76, 101	17 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	TYR	3.6
1	A	141	GLY	2.4
1	A	174	GLY	2.3
1	B	653	PRO	2.1
1	A	138	ALA	2.0
1	A	63	PRO	2.0
1	B	401	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

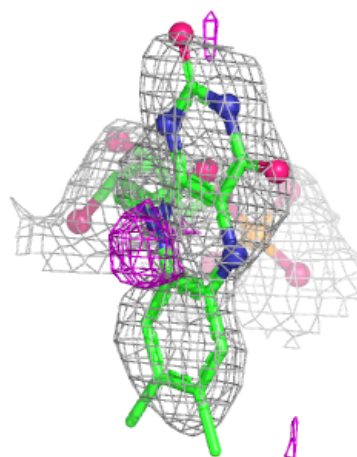
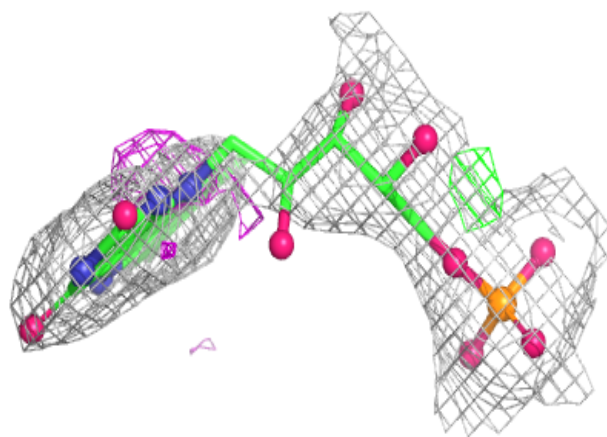
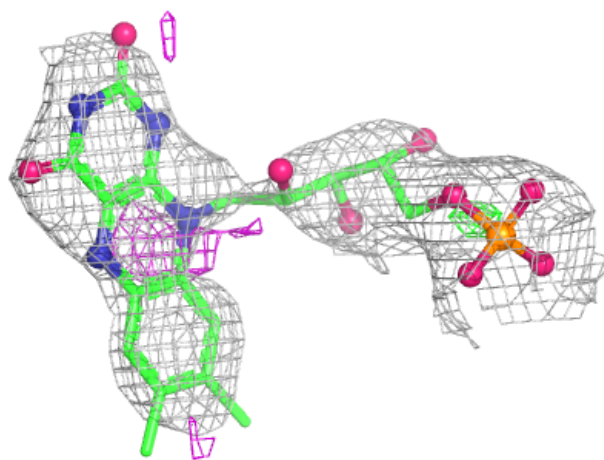
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMN	A	751	31/31	0.91	0.13	36,61,65,69	0
4	NAP	B	852	48/48	0.91	0.11	32,44,75,85	0
2	FAD	B	850	53/53	0.95	0.07	20,29,39,41	0
4	NAP	A	752	48/48	0.96	0.08	20,41,61,64	0
2	FAD	A	750	53/53	0.97	0.07	24,36,43,46	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.

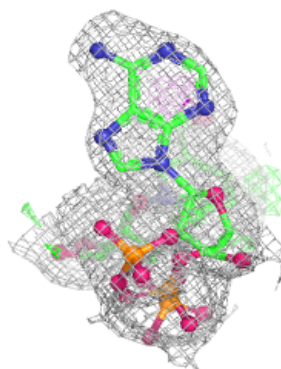
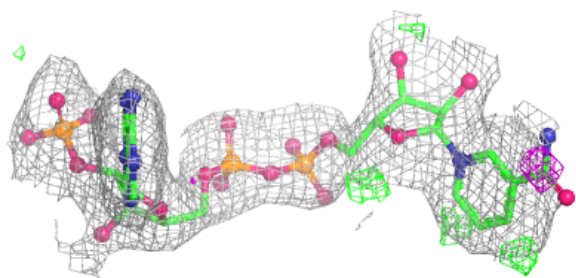
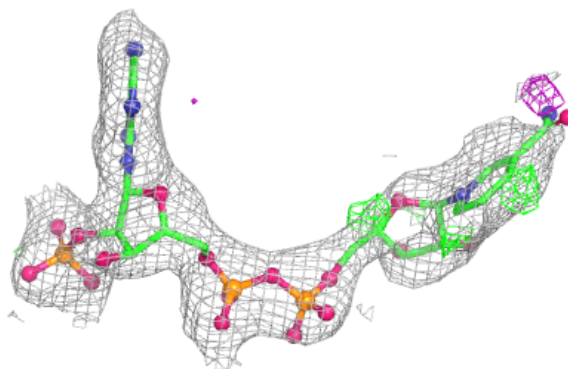
Electron density around FMN A 751:

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

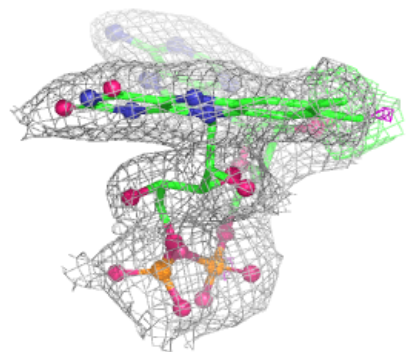
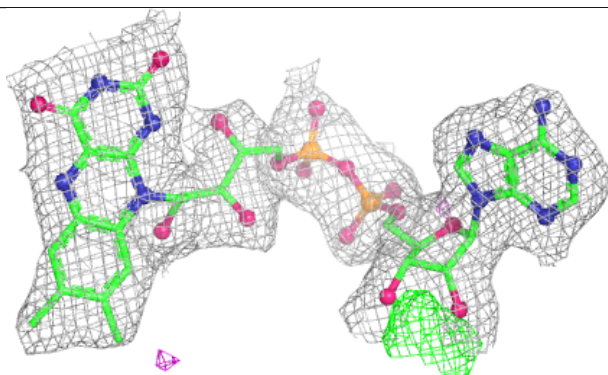
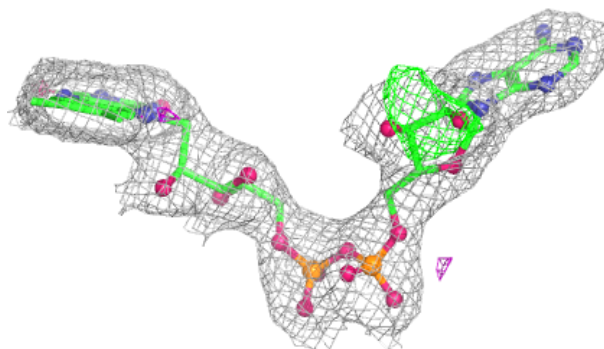


Electron density around NAP B 852:

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

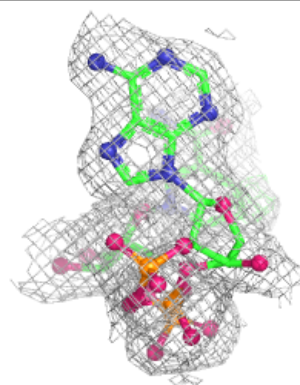
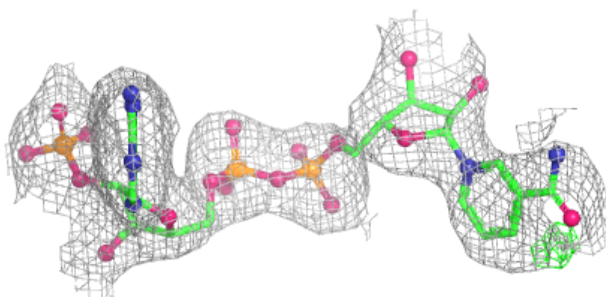
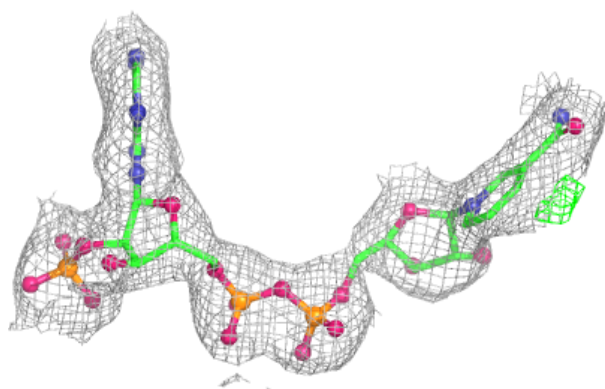
**Electron density around FAD B 850:**

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

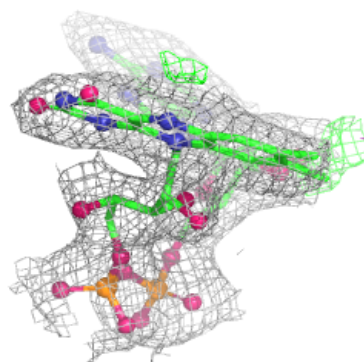
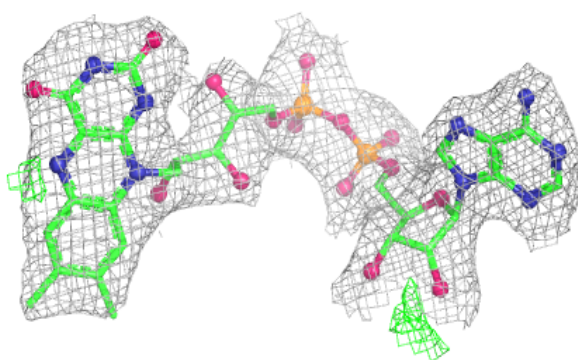
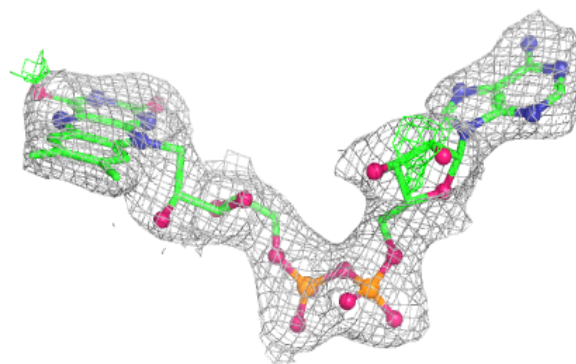


Electron density around NAP A 752:

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

**Electron density around FAD A 750:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.