



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 06:54 PM EDT

PDB ID : 5URI  
Title : Rat CYPOR/D632A with 2'-AMP  
Authors : Xia, C.; Kim, J.J.  
Deposited on : 2017-02-10  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.37.1
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)	:	2.37.1

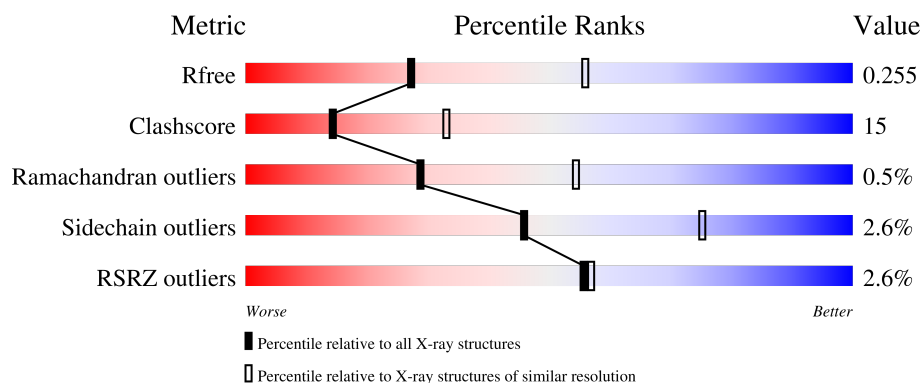
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	622	 69% 28% ..
1	B	622	 5% 64% 32% ..

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10102 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.

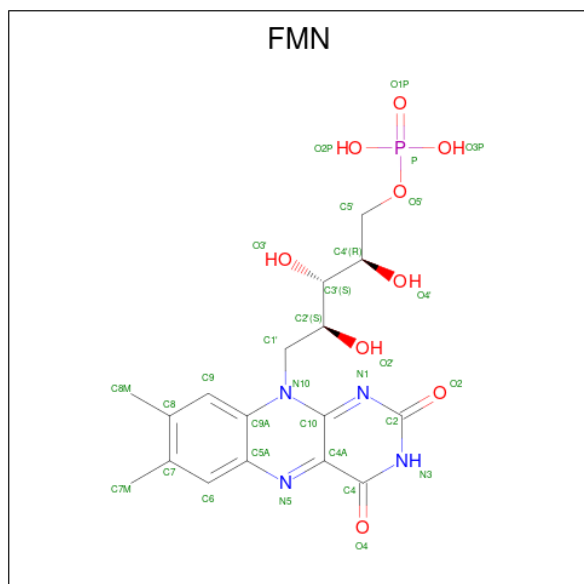
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	2
			4871	3089	836	923	23			
1	B	603	Total	C	N	O	S	0	0	1
			4778	3026	825	904	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	632	ALA	ASP	engineered mutation	UNP P00388
B	632	ALA	ASP	engineered mutation	UNP P00388

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



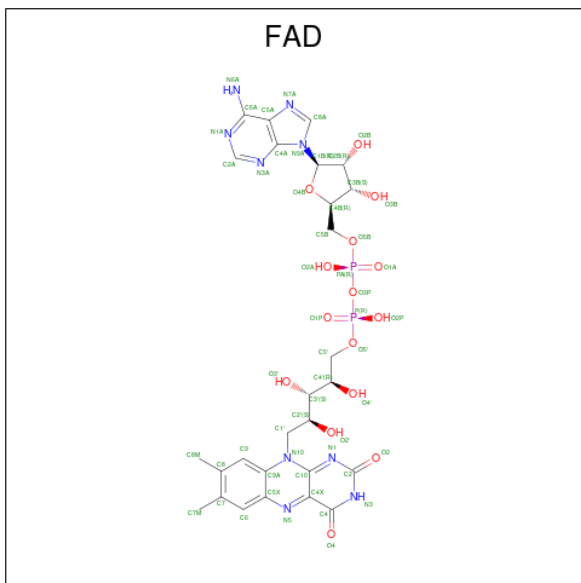
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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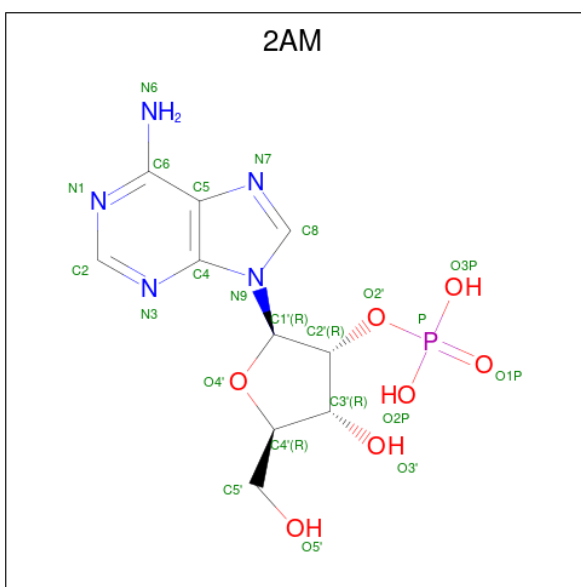
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



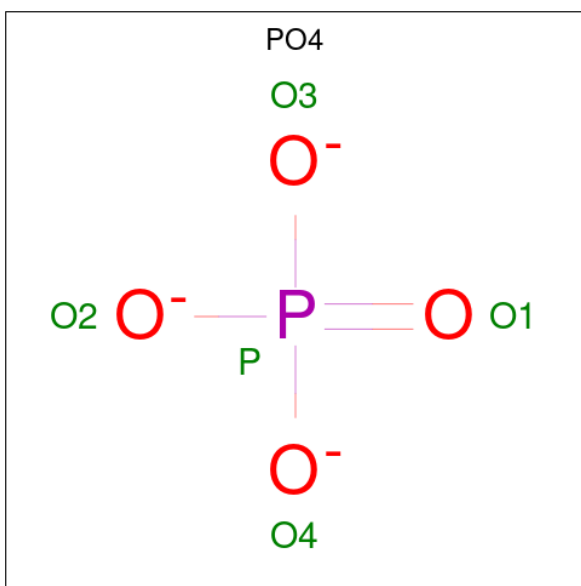
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is ADENOSINE-2'-MONOPHOSPHATE (three-letter code: 2AM) (formula:  $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_7\text{P}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

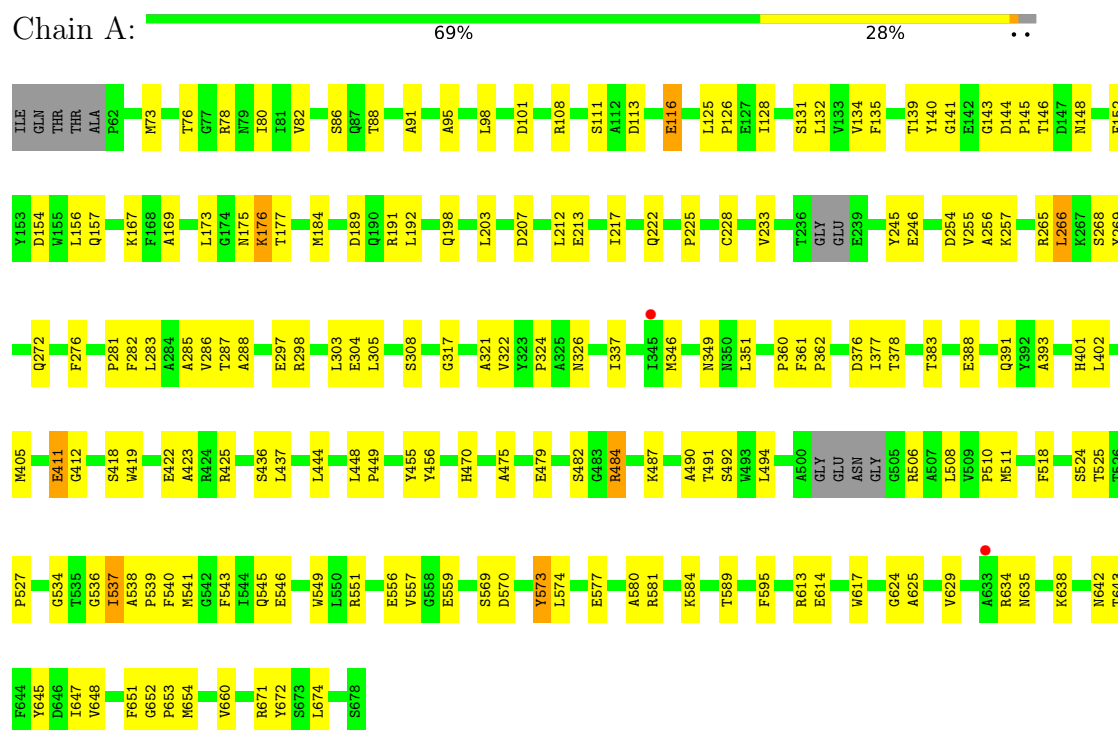
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total 135	O 135	0	0
6	B	94	Total 94	O 94	0	0

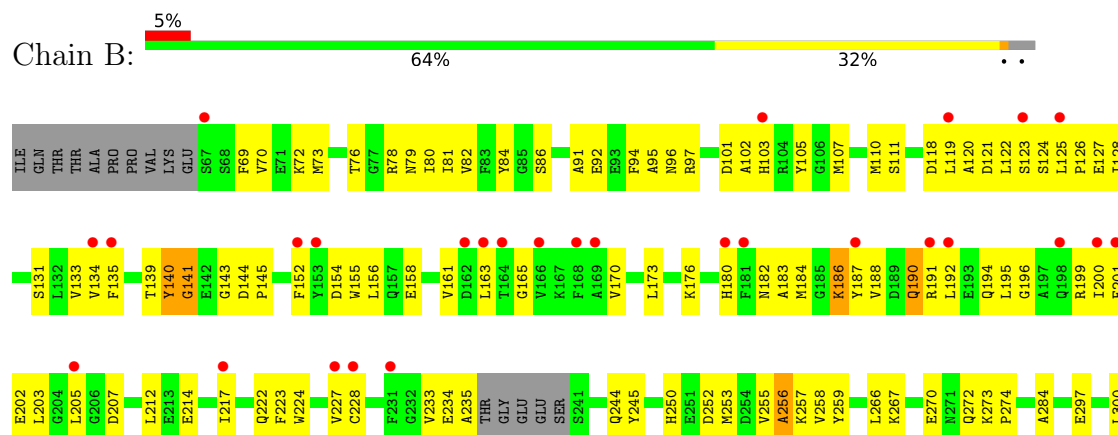
### 3 Residue-property plots

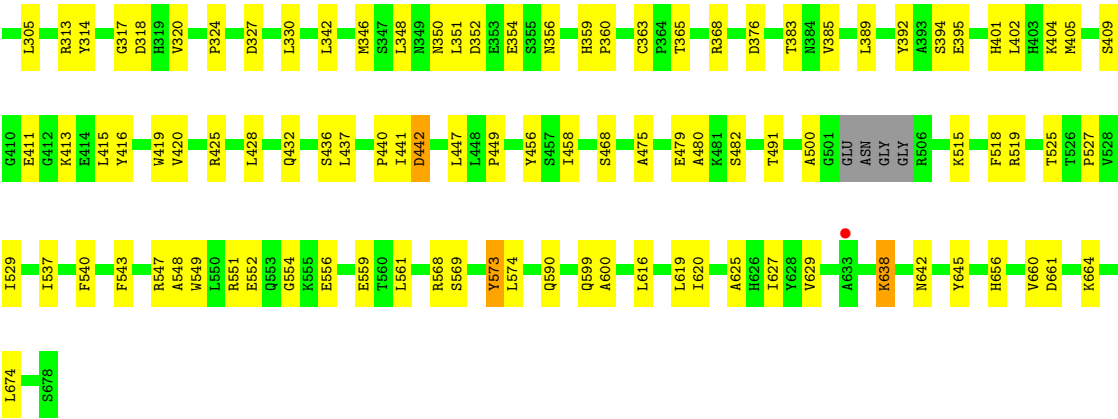
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: NADPH-cytochrome P450 reductase



#### • Molecule 1: NADPH-cytochrome P450 reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.28Å 115.81Å 117.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.26 – 2.70 38.26 – 2.69	Depositor EDS
% Data completeness (in resolution range)	96.6 (38.26-2.70) 96.1 (38.26-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.50 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.203 , 0.264 0.199 , 0.255	Depositor DCC
$R_{free}$ test set	1868 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2AM, FAD, PO4, 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	0.38	0/4987	0.61	1/6747 (0.0%)
1	B	0.36	0/4892	0.63	2/6620 (0.0%)
All	All	0.37	0/9879	0.62	3/13367 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	LEU	N-CA-CB	-6.99	96.42	110.40
1	A	537	ILE	CB-CA-C	-6.07	99.45	111.60
1	B	143	GLY	N-CA-C	5.67	127.27	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	4871	0	4711	115	0
1	B	4778	0	4570	184	0
2	A	31	0	19	1	0
2	B	31	0	19	0	0
3	A	53	0	31	1	0
3	B	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	23	0	12	1	0
4	B	23	0	12	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	135	0	0	5	0
6	B	94	0	0	10	0
All	All	10102	0	9405	298	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 15.

All (298) 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:180:HIS:HB3	1:B:183:ALA:HB2	1.36	1.03
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.40	1.00
1:B:190:GLN:N	1:B:190:GLN:HE21	1.63	0.96
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.31	0.92
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.56	0.87
1:A:581:ARG:HH21	1:A:584:LYS:HD3	1.38	0.86
1:B:409:SER:HA	1:B:413:LYS:HD2	1.57	0.85
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.60	0.84
1:B:163:LEU:O	1:B:196:GLY:HA3	1.80	0.81
1:B:79:ASN:ND2	1:B:80:ILE:HG13	1.96	0.81
1:B:199:ARG:HD3	1:B:201:PHE:O	1.80	0.80
1:A:113:ASP:HB3	1:A:116:GLU:HG3	1.63	0.80
1:B:359:HIS:ND1	1:B:363:CYS:HB2	1.97	0.79
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.65	0.78
1:B:199:ARG:CG	1:B:201:PHE:O	2.32	0.77
1:A:537:ILE:HG13	1:A:537:ILE:O	1.86	0.76
1:B:70:VAL:HG23	1:B:121:ASP:HB3	1.67	0.75
1:A:581:ARG:NH2	1:A:584:LYS:HD3	2.02	0.75
1:B:186:LYS:HA	1:B:203:LEU:HD21	1.67	0.74
1:B:119:LEU:HG	1:B:152:PHE:HD1	1.52	0.74
1:B:145:PRO:HB3	1:B:184:MET:SD	2.29	0.73
1:B:190:GLN:HE21	1:B:190:GLN:H	1.37	0.72
1:A:88:THR:HB	2:A:701:FMN:O1P	1.91	0.71
1:B:428:LEU:O	1:B:432:GLN:HG3	1.91	0.70
1:B:123:SER:O	1:B:126:PRO:HD2	1.92	0.70
1:A:337:ILE:HB	1:B:600:ALA:HB1	1.74	0.69
1:B:300:LEU:HD22	1:B:574:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLU:HG2	1:A:470:HIS:CD2	2.28	0.69
1:A:614:GLU:HA	1:A:651:PHE:CE2	2.28	0.69
1:B:199:ARG:CD	1:B:201:PHE:O	2.41	0.69
1:B:176:LYS:HE3	1:B:207:ASP:HB2	1.75	0.68
1:B:190:GLN:N	1:B:190:GLN:NE2	2.40	0.68
1:B:266:LEU:HG	1:B:267:LYS:HG2	1.75	0.68
1:B:69:PHE:CE1	1:B:121:ASP:HB2	2.29	0.67
1:B:79:ASN:ND2	1:B:107:MET:HB3	2.08	0.67
1:A:527:PRO:HB2	1:A:625:ALA:CB	2.25	0.67
1:A:78:ARG:HG2	1:A:78:ARG:HH11	1.61	0.66
1:B:313:ARG:HA	6:B:861:HOH:O	1.94	0.65
1:B:122:LEU:HD12	1:B:155:TRP:HZ3	1.60	0.65
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.77	0.65
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.77	0.65
1:A:541:MET:O	1:A:545:GLN:HG3	1.95	0.65
1:B:385:VAL:HG13	1:B:447:LEU:HB3	1.79	0.64
1:B:70:VAL:CG2	1:B:121:ASP:HB3	2.28	0.64
1:A:634:ARG:O	1:A:638:LYS:HG2	1.98	0.63
1:B:184:MET:O	1:B:188:VAL:HG23	1.97	0.63
1:A:82:VAL:HG22	1:A:134:VAL:HB	1.81	0.63
1:A:246:GLU:HB3	1:A:351:LEU:HD21	1.80	0.63
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.81	0.63
1:B:234:GLU:HG3	1:B:235:ALA:H	1.63	0.63
1:B:250:HIS:HB3	1:B:253:MET:HB3	1.79	0.62
1:B:119:LEU:HG	1:B:152:PHE:CD1	2.33	0.62
1:B:122:LEU:HD12	1:B:155:TRP:CZ3	2.34	0.62
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.82	0.61
1:B:81:ILE:HA	1:B:110:MET:O	2.01	0.61
1:B:188:VAL:O	1:B:192:LEU:HG	1.99	0.61
1:B:257:LYS:O	1:B:257:LYS:HG2	1.99	0.61
1:A:559:GLU:HG2	1:A:589:THR:HG21	1.82	0.60
1:B:255:VAL:HG23	1:B:256:ALA:N	2.15	0.60
1:A:642:ASN:HA	1:A:645:TYR:CD2	2.37	0.60
1:B:214:GLU:OE1	1:B:214:GLU:HA	2.02	0.60
1:A:175:ASN:OD1	1:A:177:THR:HG23	2.02	0.59
1:A:444:LEU:O	1:A:448:LEU:HG	2.02	0.59
1:B:661:ASP:HA	1:B:664:LYS:HB2	1.85	0.59
1:A:475:ALA:HA	1:A:491:THR:HB	1.85	0.58
1:B:186:LYS:O	1:B:190:GLN:NE2	2.36	0.58
1:B:480:ALA:C	1:B:482:SER:H	2.06	0.58
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:TYR:CE2	1:B:458:ILE:HG21	2.39	0.57
1:A:525:THR:HG22	1:A:556:GLU:HG2	1.86	0.57
1:A:645:TYR:CE1	1:A:660:VAL:HA	2.39	0.57
1:A:402:LEU:HD11	1:A:437:LEU:HD22	1.87	0.57
1:B:217:ILE:HD11	1:B:383:THR:OG1	2.05	0.56
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.88	0.56
1:A:423:ALA:O	1:A:482:SER:HB3	2.06	0.56
1:A:285:ALA:HA	1:A:508:LEU:HD23	1.88	0.56
1:B:201:PHE:CD2	1:B:223:PHE:HA	2.41	0.55
1:B:223:PHE:O	1:B:227:VAL:HG23	2.07	0.55
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.70	0.55
1:A:624:GLY:HA2	1:A:671:ARG:NH2	2.21	0.55
1:A:326:ASN:HB3	1:A:377:ILE:HD11	1.87	0.55
1:A:534:GLY:HA3	4:A:703:2AM:H5'1	1.89	0.55
1:B:629:VAL:HB	1:B:674:LEU:CD2	2.36	0.55
1:A:139:THR:CG2	1:A:143:GLY:HA2	2.37	0.55
1:B:419:TRP:O	1:B:425:ARG:HD2	2.06	0.55
1:B:559:GLU:OE2	1:B:619:LEU:HD21	2.07	0.55
1:A:139:THR:HG21	1:A:143:GLY:HA2	1.89	0.55
1:B:69:PHE:O	1:B:73:MET:HG3	2.07	0.55
1:B:629:VAL:HB	1:B:674:LEU:HD23	1.89	0.55
1:B:475:ALA:HA	1:B:491:THR:HB	1.89	0.55
1:B:176:LYS:HE3	1:B:207:ASP:CB	2.37	0.54
1:A:88:THR:HG22	1:A:88:THR:O	2.07	0.54
1:B:133:VAL:O	1:B:133:VAL:HG13	2.06	0.54
1:B:548:ALA:O	1:B:552:GLU:HG3	2.07	0.54
1:B:645:TYR:CE1	1:B:660:VAL:HA	2.42	0.54
1:A:82:VAL:O	1:A:111:SER:HA	2.08	0.54
1:B:182:ASN:OD1	1:B:205:LEU:HB3	2.07	0.54
1:A:269:TYR:CD1	1:A:283:LEU:HD11	2.42	0.53
1:B:76:THR:O	1:B:76:THR:HG22	2.08	0.53
1:B:405:MET:HE3	1:B:415:LEU:HD23	1.89	0.53
1:B:82:VAL:HG13	1:B:134:VAL:HB	1.89	0.53
1:B:416:TYR:O	1:B:420:VAL:HB	2.08	0.53
1:B:76:THR:HB	1:B:78:ARG:HG2	1.91	0.53
1:B:529:ILE:HD13	1:B:616:LEU:HD22	1.90	0.53
1:B:537:ILE:O	1:B:537:ILE:HG13	2.08	0.53
1:B:69:PHE:CZ	1:B:121:ASP:HB2	2.44	0.52
1:B:125:LEU:N	1:B:126:PRO:HD2	2.24	0.52
1:B:402:LEU:HD11	1:B:437:LEU:HD22	1.91	0.52
1:A:378:THR:HB	6:A:927:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:CYS:HB3	1:B:233:VAL:O	2.10	0.52
1:A:269:TYR:HE1	1:A:281:PRO:HG2	1.74	0.52
1:A:276:PHE:CG	1:A:282:PHE:HB2	2.45	0.52
1:B:86:SER:CB	1:B:91:ALA:HB3	2.27	0.52
1:A:135:PHE:CE2	1:A:192:LEU:HD11	2.45	0.52
1:B:327:ASP:HB3	1:B:330:LEU:HB2	1.92	0.52
1:A:418:SER:HA	1:A:422:GLU:HB3	1.90	0.52
1:B:144:ASP:HB3	1:B:145:PRO:HD2	1.91	0.52
1:B:547:ARG:O	1:B:551:ARG:HG3	2.10	0.52
1:B:642:ASN:HA	1:B:645:TYR:CD2	2.45	0.52
1:A:506:ARG:O	1:A:508:LEU:HG	2.09	0.52
1:B:186:LYS:NZ	1:B:186:LYS:HB3	2.25	0.52
1:B:201:PHE:CE1	1:B:202:GLU:HG2	2.44	0.51
1:B:233:VAL:HG22	1:B:234:GLU:H	1.74	0.51
1:B:170:VAL:O	1:B:203:LEU:HD12	2.10	0.51
1:B:500:ALA:HA	6:B:889:HOH:O	2.10	0.51
1:B:101:ASP:HB2	1:B:224:TRP:CZ2	2.46	0.50
1:B:190:GLN:HE21	1:B:190:GLN:CA	2.23	0.50
1:B:297:GLU:OE1	1:B:568:ARG:NH1	2.42	0.50
1:A:349:ASN:HB3	6:A:843:HOH:O	2.11	0.50
1:B:320:VAL:HG12	1:B:456:TYR:O	2.12	0.50
1:A:213:GLU:O	1:A:217:ILE:HG13	2.11	0.50
1:B:190:GLN:O	1:B:194:GLN:HG2	2.12	0.50
1:B:389:LEU:HD21	1:B:447:LEU:HD12	1.93	0.50
1:B:266:LEU:O	1:B:267:LYS:HB2	2.12	0.50
1:B:561:LEU:CD2	1:B:590:GLN:HB2	2.39	0.50
1:B:342:LEU:HB2	1:B:368:ARG:NH2	2.26	0.50
1:B:173:LEU:N	1:B:173:LEU:HD12	2.28	0.49
1:B:199:ARG:HG3	1:B:201:PHE:O	2.12	0.49
1:B:549:TRP:HA	1:B:552:GLU:HG3	1.94	0.49
1:B:401:HIS:O	1:B:405:MET:HG2	2.12	0.49
1:B:404:LYS:NZ	1:B:411:GLU:HB3	2.27	0.49
1:B:480:ALA:C	1:B:482:SER:N	2.66	0.49
1:B:620:ILE:HD11	1:B:627:ILE:HD11	1.95	0.49
1:B:233:VAL:HG22	1:B:234:GLU:N	2.28	0.49
1:A:317:GLY:HA3	1:A:518:PHE:O	2.12	0.48
1:A:411:GLU:HG3	1:A:412:GLY:N	2.28	0.48
1:B:258:VAL:CG1	1:B:365:THR:HA	2.43	0.48
1:A:288:ALA:O	1:A:303:LEU:HA	2.14	0.48
1:A:546:GLU:O	1:A:549:TRP:HB3	2.14	0.48
1:B:201:PHE:CD1	1:B:202:GLU:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ASP:OD1	1:B:515:LYS:HA	2.13	0.48
1:B:245:TYR:CD2	1:B:360:PRO:HD3	2.48	0.48
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.79	0.48
1:A:140:TYR:O	1:A:144:ASP:HB2	2.14	0.48
1:B:70:VAL:HG21	1:B:124:SER:HB2	1.96	0.48
1:A:484:ARG:N	1:A:484:ARG:HD2	2.28	0.48
1:B:186:LYS:HA	1:B:203:LEU:CD2	2.38	0.48
1:A:217:ILE:HD11	1:A:383:THR:HG21	1.95	0.47
1:A:228:CYS:HA	1:A:233:VAL:CG2	2.43	0.47
1:A:401:HIS:O	1:A:405:MET:HG2	2.13	0.47
1:A:569:SER:HB3	1:A:595:PHE:CZ	2.49	0.47
1:B:201:PHE:CD1	1:B:202:GLU:HG2	2.49	0.47
1:B:255:VAL:O	1:B:257:LYS:N	2.48	0.47
1:A:140:TYR:CD1	1:A:146:THR:HG22	2.50	0.47
1:B:297:GLU:CD	1:B:568:ARG:HH11	2.17	0.47
1:A:145:PRO:HG3	1:A:184:MET:SD	2.54	0.47
1:B:76:THR:HG22	1:B:78:ARG:HE	1.80	0.47
1:B:187:TYR:HB2	6:B:841:HOH:O	2.15	0.47
1:B:76:THR:HG21	1:B:352:ASP:OD2	2.15	0.47
1:B:73:MET:CA	1:B:78:ARG:HB2	2.44	0.47
1:B:270:GLU:CB	6:B:837:HOH:O	2.63	0.47
1:A:173:LEU:HD23	1:A:212:LEU:HD21	1.97	0.47
1:A:393:ALA:HA	1:A:436:SER:O	2.15	0.47
1:A:536:GLY:O	1:A:539:PRO:HD2	2.14	0.47
1:B:638:LYS:HB2	1:B:638:LYS:NZ	2.29	0.47
1:A:490:ALA:O	1:A:494:LEU:HG	2.15	0.46
1:A:652:GLY:N	1:A:653:PRO:HA	2.31	0.46
1:B:72:LYS:HG2	1:B:354:GLU:HB3	1.98	0.46
1:B:234:GLU:OE2	1:B:234:GLU:HA	2.14	0.46
1:A:581:ARG:HE	1:A:581:ARG:HA	1.81	0.46
1:B:200:ILE:HG22	1:B:200:ILE:O	2.15	0.46
1:B:405:MET:HE1	1:B:415:LEU:HB3	1.97	0.46
1:A:255:VAL:HG23	1:A:256:ALA:N	2.30	0.46
1:B:201:PHE:CE2	1:B:223:PHE:HA	2.50	0.46
1:B:267:LYS:HD3	6:B:837:HOH:O	2.14	0.46
1:B:70:VAL:HG11	1:B:124:SER:HB3	1.96	0.46
1:B:140:TYR:O	1:B:141:GLY:O	2.34	0.46
1:B:128:ILE:O	1:B:131:SER:OG	2.34	0.46
1:B:186:LYS:HG3	6:B:841:HOH:O	2.16	0.46
1:B:548:ALA:O	1:B:552:GLU:CG	2.64	0.46
1:B:599:GLN:N	1:B:599:GLN:CD	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:THR:CG2	1:B:78:ARG:HE	2.29	0.45
1:B:73:MET:HA	1:B:78:ARG:HB2	1.98	0.45
1:B:79:ASN:HD22	1:B:80:ILE:HG13	1.77	0.45
1:A:569:SER:HA	1:A:573:TYR:HB2	1.97	0.45
1:B:82:VAL:O	1:B:111:SER:HA	2.17	0.45
1:A:128:ILE:HB	1:A:131:SER:HB3	1.99	0.45
1:B:201:PHE:HD1	1:B:202:GLU:N	2.13	0.45
1:B:350:ASN:OD1	1:B:351:LEU:N	2.49	0.45
1:A:322:VAL:HG12	1:A:511:MET:HB3	1.99	0.45
1:A:617:TRP:HZ3	1:A:648:VAL:HG22	1.82	0.45
1:B:139:THR:HG23	1:B:183:ALA:HB3	1.98	0.45
1:A:574:LEU:HG	6:A:821:HOH:O	2.17	0.45
1:A:645:TYR:CD1	1:A:660:VAL:HA	2.51	0.45
1:B:154:ASP:O	1:B:158:GLU:N	2.49	0.45
1:B:182:ASN:O	1:B:186:LYS:HG2	2.15	0.45
1:B:519:ARG:HG2	1:B:519:ARG:HH11	1.81	0.45
1:A:78:ARG:HG2	1:A:78:ARG:NH1	2.31	0.45
1:A:98:LEU:O	1:A:101:ASP:HB2	2.17	0.44
1:A:297:GLU:C	1:A:298:ARG:HG3	2.37	0.44
1:B:126:PRO:HB3	1:B:165:GLY:O	2.17	0.44
1:B:234:GLU:HG3	1:B:235:ALA:N	2.30	0.44
1:B:134:VAL:HG12	1:B:135:PHE:N	2.33	0.44
1:B:84:TYR:HB3	1:B:95:ALA:HB2	1.99	0.44
1:B:80:ILE:HD11	1:B:107:MET:SD	2.56	0.44
1:B:214:GLU:OE1	1:B:217:ILE:HD12	2.18	0.44
1:A:125:LEU:N	1:A:126:PRO:CD	2.81	0.44
1:B:190:GLN:NE2	1:B:190:GLN:CA	2.80	0.44
1:B:201:PHE:HD1	1:B:202:GLU:H	1.63	0.44
1:B:395:GLU:HB3	1:B:436:SER:OG	2.17	0.44
1:A:189:ASP:HB2	1:A:203:LEU:HD13	1.99	0.44
1:A:556:GLU:HB2	6:A:934:HOH:O	2.16	0.44
1:B:118:ASP:C	1:B:120:ALA:H	2.20	0.44
1:B:441:ILE:HG23	1:B:442:ASP:N	2.33	0.44
1:B:255:VAL:C	1:B:257:LYS:N	2.70	0.44
1:B:320:VAL:HG13	1:B:320:VAL:O	2.18	0.44
1:A:643:THR:O	1:A:647:ILE:HG13	2.18	0.43
1:B:92:GLU:HG2	1:B:96:ASN:HD21	1.83	0.43
1:B:525:THR:HG22	1:B:556:GLU:O	2.18	0.43
1:A:653:PRO:O	1:A:654:MET:HB3	2.18	0.43
1:B:552:GLU:C	1:B:554:GLY:H	2.20	0.43
1:B:94:PHE:O	1:B:95:ALA:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLN:OE1	1:A:282:PHE:HA	2.17	0.43
1:B:305:LEU:O	1:B:468:SER:HA	2.18	0.43
1:A:152:PHE:CE1	1:A:156:LEU:HD21	2.53	0.43
1:A:257:LYS:HA	1:A:266:LEU:HD21	2.00	0.43
1:B:284:ALA:HA	6:B:857:HOH:O	2.18	0.43
1:A:76:THR:OG1	1:A:78:ARG:HG3	2.18	0.43
1:B:270:GLU:HB2	6:B:837:HOH:O	2.18	0.43
1:A:419:TRP:O	1:A:425:ARG:HD2	2.18	0.43
1:A:613:ARG:HG2	1:A:613:ARG:NH1	2.32	0.43
1:A:308:SER:HA	6:A:817:HOH:O	2.19	0.42
1:A:456:TYR:HH	3:A:702:FAD:HO4'	1.67	0.42
1:B:102:ALA:O	1:B:105:TYR:N	2.51	0.42
1:B:244:GLN:O	1:B:244:GLN:HG3	2.19	0.42
1:B:569:SER:HA	1:B:573:TYR:HB2	2.01	0.42
1:A:134:VAL:HG22	1:A:169:ALA:HB3	2.00	0.42
1:A:167:LYS:NZ	1:A:198:GLN:OE1	2.51	0.42
1:B:317:GLY:HA3	1:B:518:PHE:O	2.19	0.42
1:B:519:ARG:HG2	1:B:519:ARG:NH1	2.34	0.42
1:A:538:ALA:HB3	1:A:539:PRO:CD	2.48	0.42
1:A:540:PHE:HA	1:A:543:PHE:HB2	2.01	0.42
1:B:119:LEU:O	1:B:122:LEU:HG	2.20	0.42
1:B:273:LYS:HA	1:B:274:PRO:HD3	1.78	0.42
1:B:656:HIS:O	1:B:660:VAL:HG23	2.18	0.42
1:B:103:HIS:C	1:B:105:TYR:H	2.23	0.42
1:B:214:GLU:OE2	1:B:413:LYS:HG3	2.20	0.42
1:B:540:PHE:HA	1:B:543:PHE:HB2	2.00	0.42
1:A:569:SER:HB3	1:A:595:PHE:CE1	2.54	0.42
1:B:125:LEU:C	1:B:127:GLU:H	2.22	0.42
1:B:352:ASP:C	1:B:354:GLU:H	2.23	0.42
1:A:286:VAL:HG22	1:A:305:LEU:CD2	2.50	0.42
1:B:140:TYR:O	1:B:141:GLY:C	2.57	0.42
1:B:267:LYS:CD	6:B:837:HOH:O	2.66	0.42
1:B:272:GLN:N	6:B:801:HOH:O	2.37	0.42
1:B:187:TYR:CE1	1:B:191:ARG:HB2	2.55	0.42
1:B:245:TYR:CE2	1:B:360:PRO:HD3	2.55	0.42
1:B:154:ASP:C	1:B:156:LEU:N	2.71	0.42
1:A:152:PHE:CZ	1:A:156:LEU:HD11	2.56	0.41
1:A:245:TYR:CD1	1:A:360:PRO:HD3	2.55	0.41
1:A:245:TYR:CE1	1:A:360:PRO:HD3	2.55	0.41
1:A:222:GLN:C	1:A:225:PRO:HD2	2.40	0.41
1:B:94:PHE:O	1:B:97:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PRO:HA	1:B:131:SER:OG	2.20	0.41
1:A:283:LEU:HG	1:A:510:PRO:HG3	2.03	0.41
1:B:105:TYR:HB3	1:B:228:CYS:SG	2.60	0.41
1:A:82:VAL:HG11	1:A:95:ALA:HA	2.03	0.41
1:A:321:ALA:HB2	1:A:455:TYR:CE2	2.56	0.41
1:A:265:ARG:O	1:A:268:SER:HB2	2.20	0.41
1:B:123:SER:C	1:B:125:LEU:H	2.24	0.41
1:A:154:ASP:O	1:A:157:GLN:HB2	2.21	0.41
1:A:176:LYS:HG3	1:A:207:ASP:CG	2.41	0.41
1:A:388:GLU:O	1:A:391:GLN:HG2	2.20	0.41
1:A:487:LYS:HE2	1:A:492:SER:OG	2.21	0.41
1:A:577:GLU:O	1:A:580:ALA:HB3	2.21	0.41
1:B:105:TYR:C	1:B:107:MET:H	2.24	0.41
1:B:255:VAL:O	1:B:258:VAL:N	2.46	0.41
1:A:80:ILE:HD12	1:A:132:LEU:HD23	2.03	0.41
1:A:573:TYR:C	1:A:573:TYR:CD1	2.94	0.41
1:B:201:PHE:HE2	1:B:222:GLN:C	2.24	0.40
1:B:259:TYR:CE1	1:B:266:LEU:HA	2.56	0.40
1:B:392:TYR:CD1	1:B:440:PRO:HD3	2.56	0.40
1:A:361:PHE:HB2	1:A:362:PRO:HD2	2.03	0.40
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.51	0.40
1:B:348:LEU:HD23	1:B:348:LEU:HA	1.94	0.40
1:A:524:SER:O	1:A:557:VAL:HA	2.21	0.40
1:A:573:TYR:C	1:A:573:TYR:HD1	2.25	0.40
1:A:73:MET:HG2	1:A:78:ARG:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	603/622 (97%)	573 (95%)	28 (5%)	2 (0%)	41 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	595/622 (96%)	521 (88%)	70 (12%)	4 (1%)	22	46
All	All	1198/1244 (96%)	1094 (91%)	98 (8%)	6 (0%)	29	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	GLY
1	B	141	GLY
1	A	176	LYS
1	B	256	ALA
1	B	394	SER
1	B	161	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	518/530 (98%)	504 (97%)	14 (3%)	44	74
1	B	499/530 (94%)	487 (98%)	12 (2%)	49	77
All	All	1017/1060 (96%)	991 (97%)	26 (3%)	46	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	148	ASN
1	A	254	ASP
1	A	266	LEU
1	A	287	THR
1	A	324	PRO
1	A	346	MET
1	A	411	GLU
1	A	479	GLU
1	A	484	ARG

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Mol	Chain	Res	Type
1	A	570	ASP
1	A	573	TYR
1	A	635	ASN
1	A	672	TYR
1	B	140	TYR
1	B	186	LYS
1	B	190	GLN
1	B	212	LEU
1	B	252	ASP
1	B	324	PRO
1	B	346	MET
1	B	356	ASN
1	B	442	ASP
1	B	479	GLU
1	B	573	TYR
1	B	638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	399	GLN
1	A	470	HIS
1	A	486	ASN
1	A	635	ASN
1	B	190	GLN
1	B	467	ASN
1	B	615	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	2AM	B	703	-	21,25,25	1.82	5 (23%)	24,38,38	1.92	3 (12%)
2	FMN	A	701	-	33,33,33	2.62	13 (39%)	48,50,50	1.58	13 (27%)
4	2AM	A	703	-	21,25,25	1.83	5 (23%)	24,38,38	1.98	4 (16%)
5	PO4	A	704	-	4,4,4	1.69	0	6,6,6	0.43	0
5	PO4	B	704	-	4,4,4	1.63	0	6,6,6	0.42	0
3	FAD	B	702	-	53,58,58	2.13	11 (20%)	68,89,89	1.52	11 (16%)
2	FMN	B	701	-	33,33,33	2.66	12 (36%)	48,50,50	1.66	13 (27%)
3	FAD	A	702	-	53,58,58	2.13	11 (20%)	68,89,89	1.52	11 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2AM	B	703	-	-	1/7/27/27	0/3/3/3
2	FMN	A	701	-	-	0/18/18/18	0/3/3/3
4	2AM	A	703	-	-	3/7/27/27	0/3/3/3
3	FAD	B	702	-	-	0/30/50/50	0/6/6/6
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3
3	FAD	A	702	-	-	0/30/50/50	0/6/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C8A-N7A	7.57	1.48	1.34
3	B	702	FAD	C8A-N7A	7.54	1.48	1.34
2	A	701	FMN	C8M-C8	-6.49	1.38	1.51
2	B	701	FMN	C8M-C8	-6.42	1.38	1.51
2	B	701	FMN	C4A-N5	5.92	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FMN	C4A-N5	5.79	1.42	1.30
3	A	702	FAD	C7M-C7	-5.76	1.39	1.51
3	A	702	FAD	C8M-C8	-5.75	1.39	1.51
3	B	702	FAD	C8M-C8	-5.74	1.39	1.51
3	B	702	FAD	C7M-C7	-5.72	1.39	1.51
2	B	701	FMN	C10-N10	5.35	1.49	1.37
4	B	703	2AM	C2-N3	5.15	1.40	1.32
4	A	703	2AM	C2-N3	5.14	1.40	1.32
3	B	702	FAD	C2A-N3A	5.14	1.40	1.32
2	B	701	FMN	C9-C9A	5.05	1.47	1.39
3	A	702	FAD	C2A-N3A	5.02	1.40	1.32
2	A	701	FMN	C10-N10	4.99	1.48	1.37
2	A	701	FMN	C9-C9A	4.75	1.47	1.39
2	B	701	FMN	C9A-N10	4.24	1.48	1.41
2	A	701	FMN	C9A-C5A	4.20	1.48	1.41
2	A	701	FMN	C9A-N10	4.10	1.48	1.41
2	A	701	FMN	C8-C7	3.88	1.50	1.40
2	B	701	FMN	C9A-C5A	3.87	1.47	1.41
2	B	701	FMN	C8-C7	3.77	1.50	1.40
3	A	702	FAD	C9A-N10	-3.66	1.34	1.41
3	B	702	FAD	C9A-N10	-3.65	1.34	1.41
3	A	702	FAD	C10-N1	3.53	1.40	1.33
2	B	701	FMN	C10-N1	3.52	1.40	1.33
3	B	702	FAD	C10-N1	3.49	1.40	1.33
4	A	703	2AM	C2-N1	3.48	1.40	1.33
3	A	702	FAD	C2A-N1A	3.43	1.40	1.33
4	B	703	2AM	C2-N1	3.43	1.40	1.33
3	B	702	FAD	C2A-N1A	3.42	1.40	1.33
2	A	701	FMN	C6-C5A	3.24	1.45	1.40
2	A	701	FMN	C10-N1	3.14	1.39	1.33
2	B	701	FMN	C6-C5A	2.89	1.44	1.40
4	A	703	2AM	C5-C4	-2.80	1.33	1.40
4	B	703	2AM	C5-C4	-2.79	1.33	1.40
3	B	702	FAD	C5A-C4A	-2.67	1.33	1.40
3	A	702	FAD	C5A-C4A	-2.65	1.33	1.40
3	A	702	FAD	C6A-C5A	-2.63	1.33	1.43
3	B	702	FAD	C6A-C5A	-2.61	1.33	1.43
4	B	703	2AM	C6-C5	-2.61	1.33	1.43
4	A	703	2AM	C6-C5	-2.61	1.33	1.43
3	B	702	FAD	C5X-N5	-2.56	1.34	1.39
3	A	702	FAD	C5X-N5	-2.56	1.34	1.39
2	A	701	FMN	C1'-C2'	2.56	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FMN	O2'-C2'	2.54	1.48	1.43
2	B	701	FMN	C4'-C3'	2.53	1.58	1.53
3	B	702	FAD	O4B-C1B	2.35	1.44	1.41
2	A	701	FMN	O2'-C2'	2.31	1.48	1.43
3	A	702	FAD	O4B-C1B	2.23	1.44	1.41
2	A	701	FMN	C4'-C3'	2.16	1.57	1.53
4	B	703	2AM	O4'-C1'	2.08	1.44	1.41
4	A	703	2AM	O4'-C1'	2.06	1.44	1.41
2	A	701	FMN	C6-C7	2.03	1.42	1.39
2	B	701	FMN	C7M-C7	2.00	1.55	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N3A-C2A-N1A	-7.25	117.35	128.68
3	B	702	FAD	N3A-C2A-N1A	-7.22	117.40	128.68
4	B	703	2AM	N3-C2-N1	-6.96	117.80	128.68
4	A	703	2AM	N3-C2-N1	-6.80	118.06	128.68
4	A	703	2AM	O4'-C1'-C2'	-4.13	99.42	106.59
2	B	701	FMN	C9A-C5A-N5	3.90	126.67	122.43
2	A	701	FMN	C9A-C5A-N5	3.75	126.50	122.43
3	A	702	FAD	P-O3P-PA	-3.66	120.26	132.83
2	B	701	FMN	P-O5'-C5'	3.64	128.31	118.30
2	B	701	FMN	O4'-C4'-C3'	-3.58	100.40	109.10
4	B	703	2AM	O4'-C1'-C2'	-3.44	100.61	106.59
2	A	701	FMN	O4'-C4'-C3'	-3.41	100.81	109.10
3	B	702	FAD	P-O3P-PA	-3.39	121.18	132.83
3	A	702	FAD	C4-N3-C2	-3.08	119.95	125.64
3	B	702	FAD	C5A-C6A-N6A	-3.05	115.72	120.35
3	B	702	FAD	C4-N3-C2	-3.01	120.09	125.64
3	A	702	FAD	C5A-C6A-N6A	-2.98	115.82	120.35
2	A	701	FMN	P-O5'-C5'	2.93	126.36	118.30
2	B	701	FMN	O4-C4-N3	-2.71	114.92	120.12
3	A	702	FAD	C4X-C4-N3	2.70	120.05	113.19
3	B	702	FAD	C10-C4X-N5	-2.69	119.15	124.86
3	B	702	FAD	C4X-C4-N3	2.68	119.99	113.19
2	B	701	FMN	O3P-P-O5'	-2.66	99.65	106.73
2	A	701	FMN	C8M-C8-C7	2.61	126.09	120.74
4	A	703	2AM	C5-C6-N6	-2.57	116.45	120.35
2	B	701	FMN	C5A-C9A-N10	-2.56	115.31	117.95
4	A	703	2AM	C3'-C2'-C1'	-2.55	98.09	102.89
3	A	702	FAD	C10-C4X-N5	-2.54	119.46	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FMN	O4-C4-N3	-2.53	115.26	120.12
2	B	701	FMN	C8M-C8-C7	2.49	125.83	120.74
4	B	703	2AM	C5-C6-N6	-2.44	116.64	120.35
2	B	701	FMN	C9-C9A-N10	2.39	125.06	121.84
2	A	701	FMN	C5A-N5-C4A	-2.38	114.11	118.07
2	A	701	FMN	O2P-P-O1P	2.36	119.91	110.68
3	B	702	FAD	C2B-C3B-C4B	-2.35	98.08	102.64
3	B	702	FAD	O4-C4-C4X	-2.34	120.40	126.60
2	A	701	FMN	C5A-C9A-N10	-2.30	115.58	117.95
2	A	701	FMN	C8M-C8-C9	-2.29	115.26	119.49
2	B	701	FMN	C4'-C3'-C2'	-2.29	108.60	113.36
3	A	702	FAD	O4-C4-C4X	-2.27	120.59	126.60
2	B	701	FMN	O2P-P-O1P	2.25	119.47	110.68
2	B	701	FMN	C5A-N5-C4A	-2.24	114.35	118.07
2	A	701	FMN	O3P-P-O5'	-2.24	100.78	106.73
3	A	702	FAD	C4X-C10-N10	2.23	119.73	116.48
2	A	701	FMN	C4'-C3'-C2'	-2.22	108.74	113.36
3	B	702	FAD	C9A-C5X-N5	-2.13	120.11	122.43
3	A	702	FAD	C4-C4X-C10	2.12	120.35	116.79
3	B	702	FAD	C4-C4X-C10	2.11	120.34	116.79
2	A	701	FMN	C9-C9A-N10	2.09	124.66	121.84
3	A	702	FAD	C2B-C3B-C4B	-2.09	98.59	102.64
3	B	702	FAD	C4X-C10-N1	-2.06	119.94	124.73
2	B	701	FMN	C7M-C7-C6	-2.06	115.68	119.49
2	B	701	FMN	C8M-C8-C9	-2.05	115.69	119.49
3	A	702	FAD	C4X-C10-N1	-2.05	119.97	124.73
2	A	701	FMN	C7M-C7-C6	-2.00	115.79	119.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	2AM	C2'-O2'-P-O1P
4	A	703	2AM	C2'-O2'-P-O1P
4	A	703	2AM	C2'-O2'-P-O2P
4	A	703	2AM	C2'-O2'-P-O3P

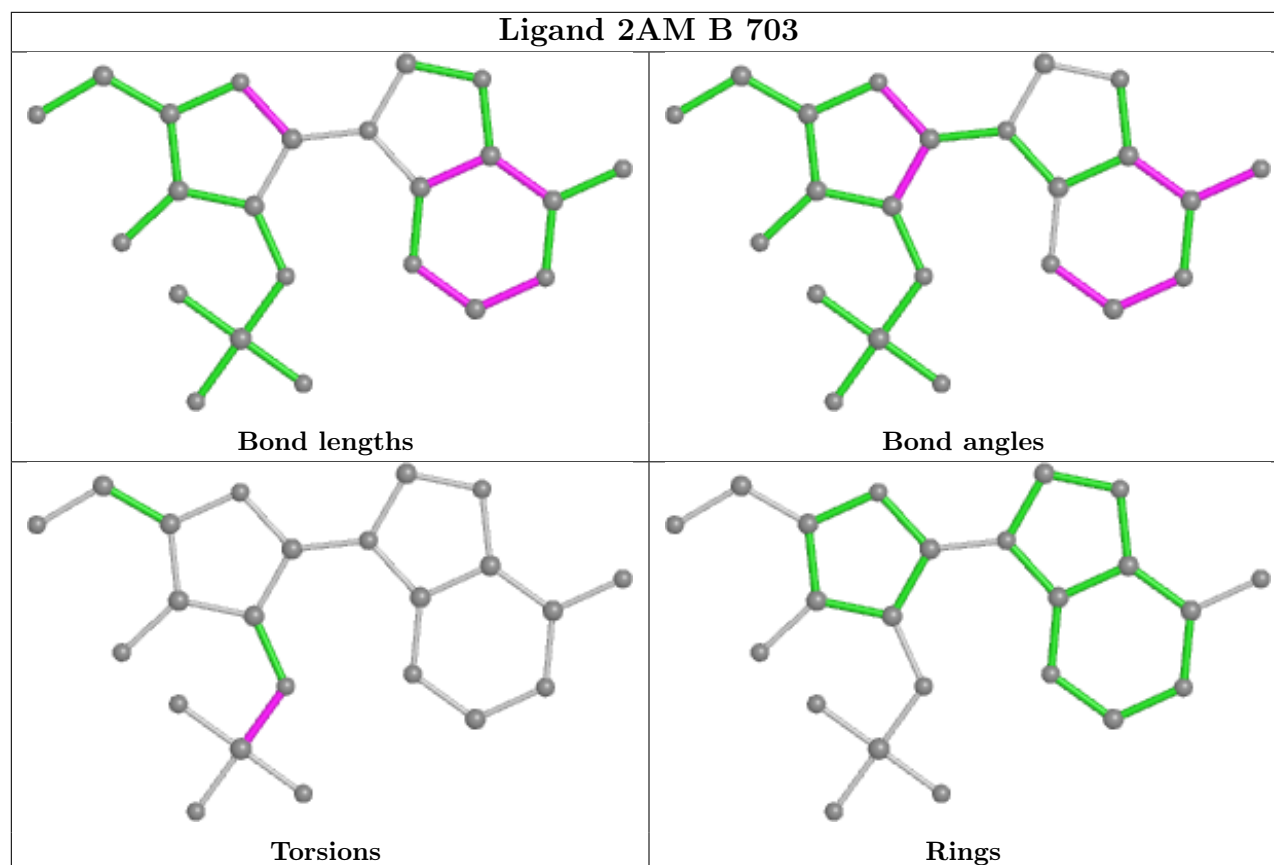
There are no ring outliers.

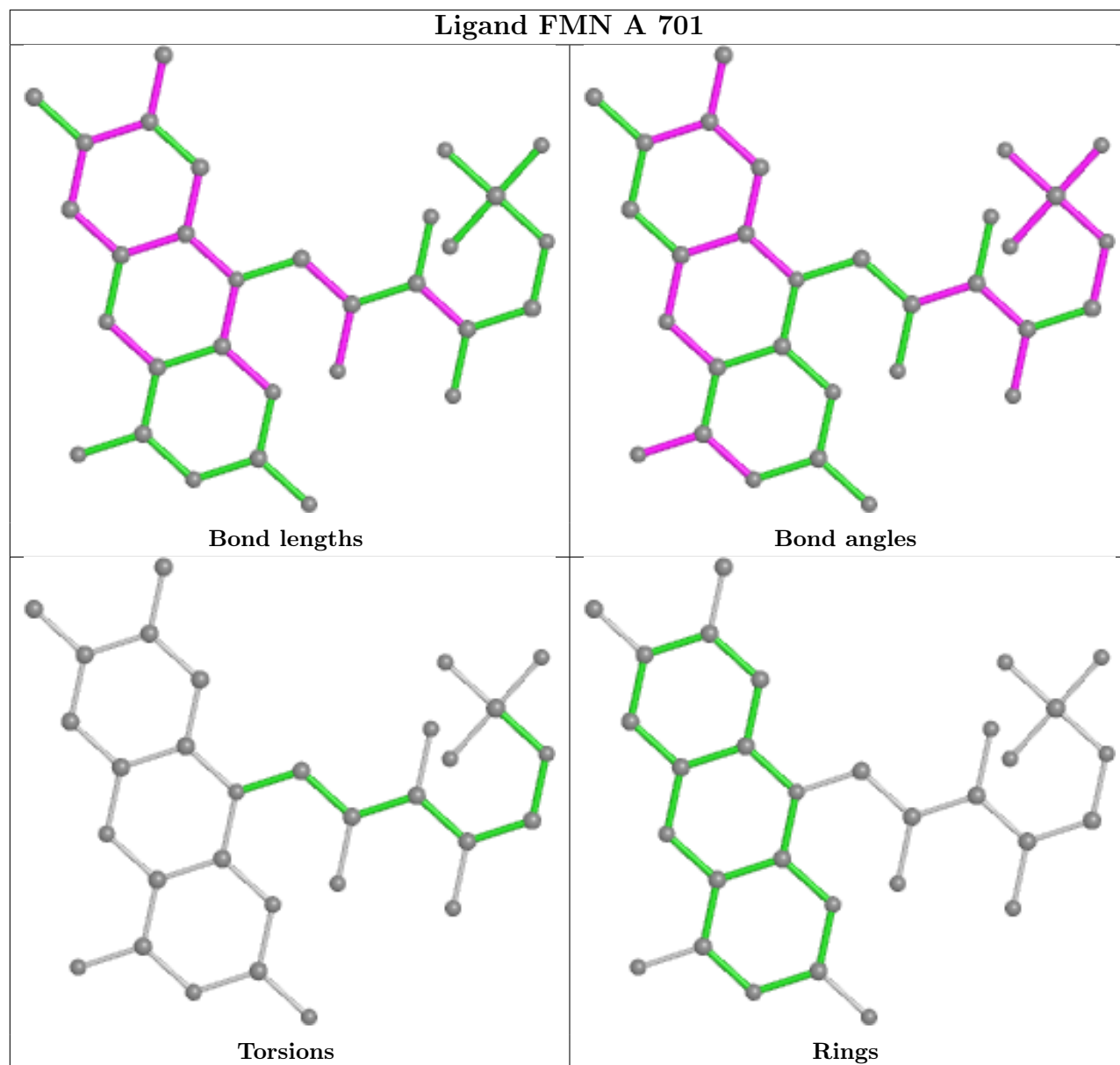
3 monomers are involved in 3 short contacts:



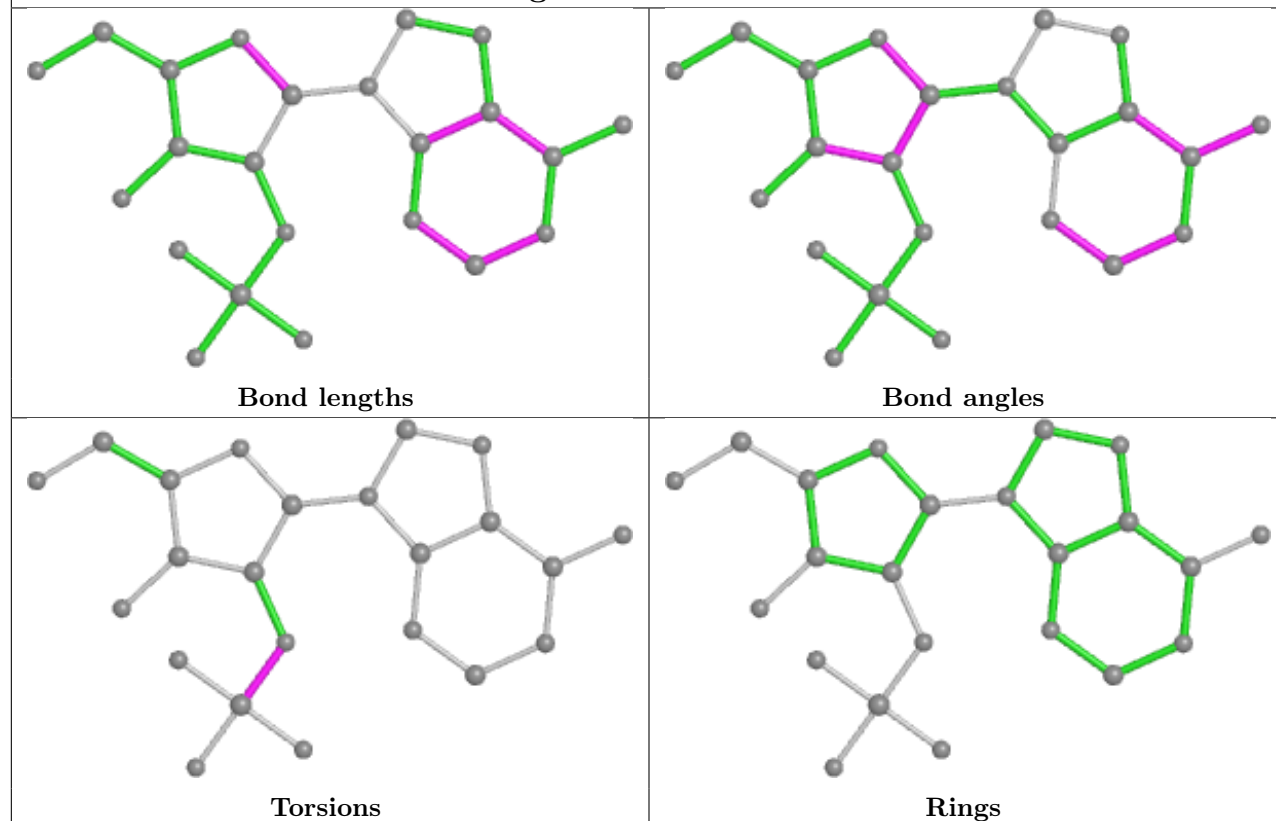
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FMN	1	0
4	A	703	2AM	1	0
3	A	702	FAD	1	0

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.

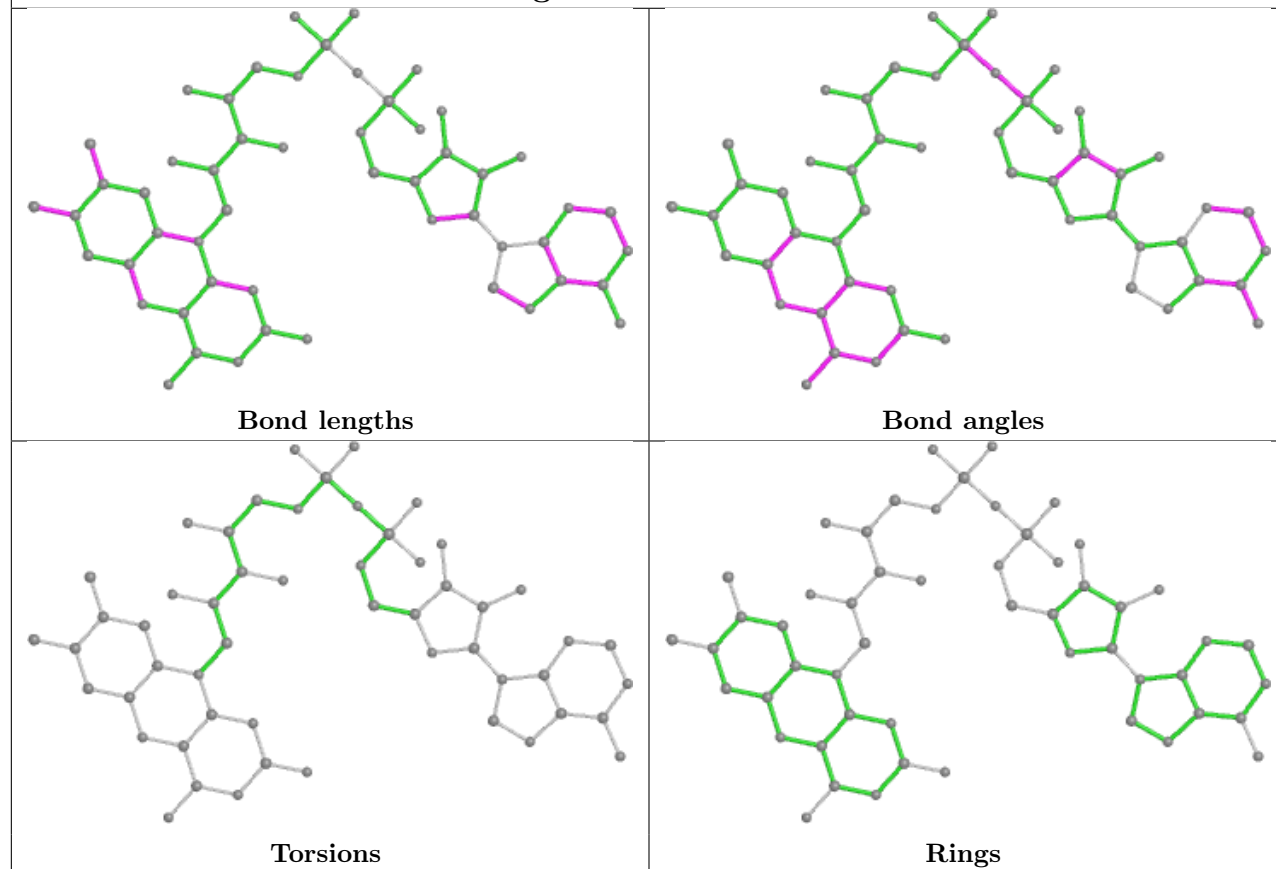


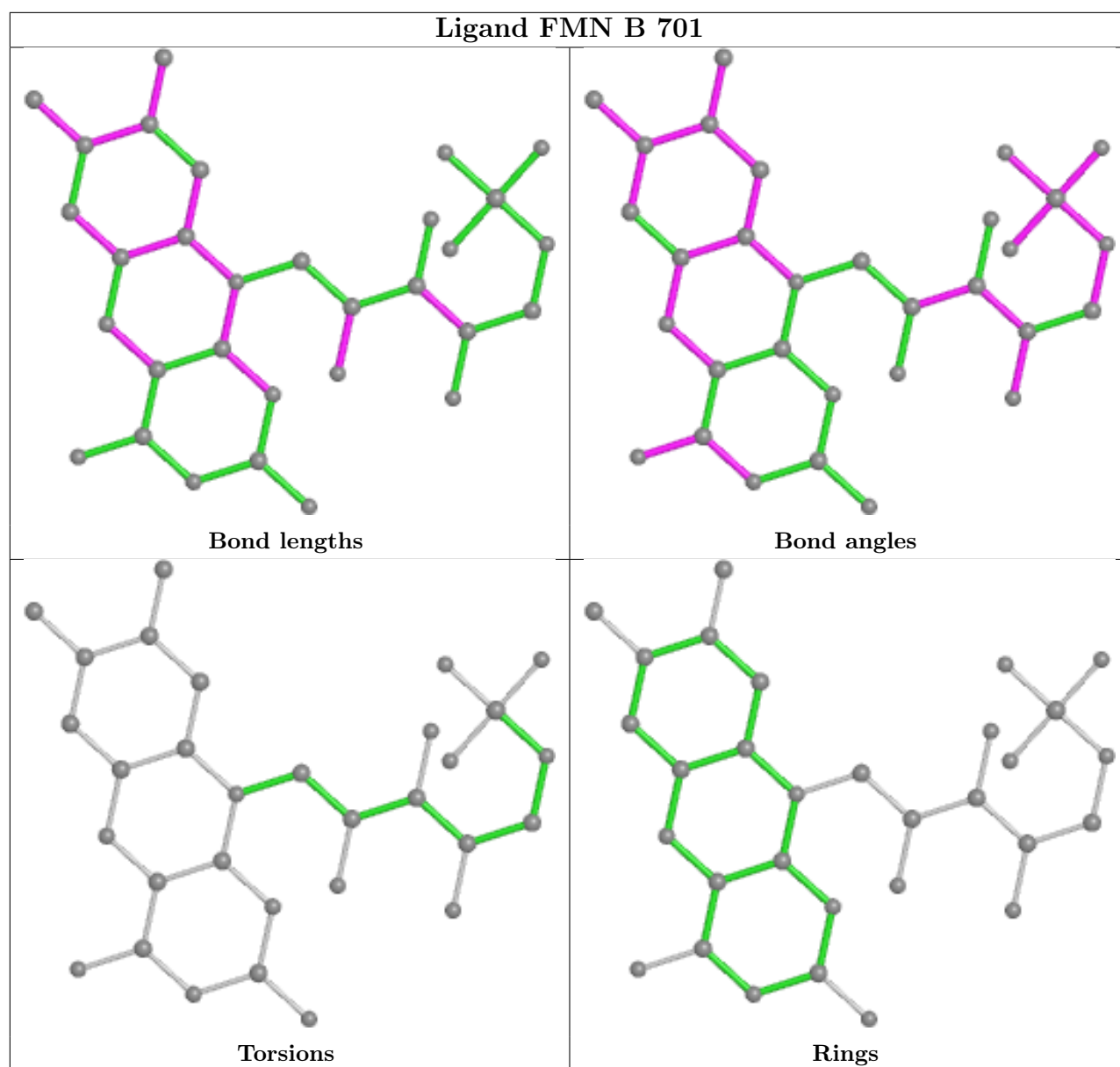


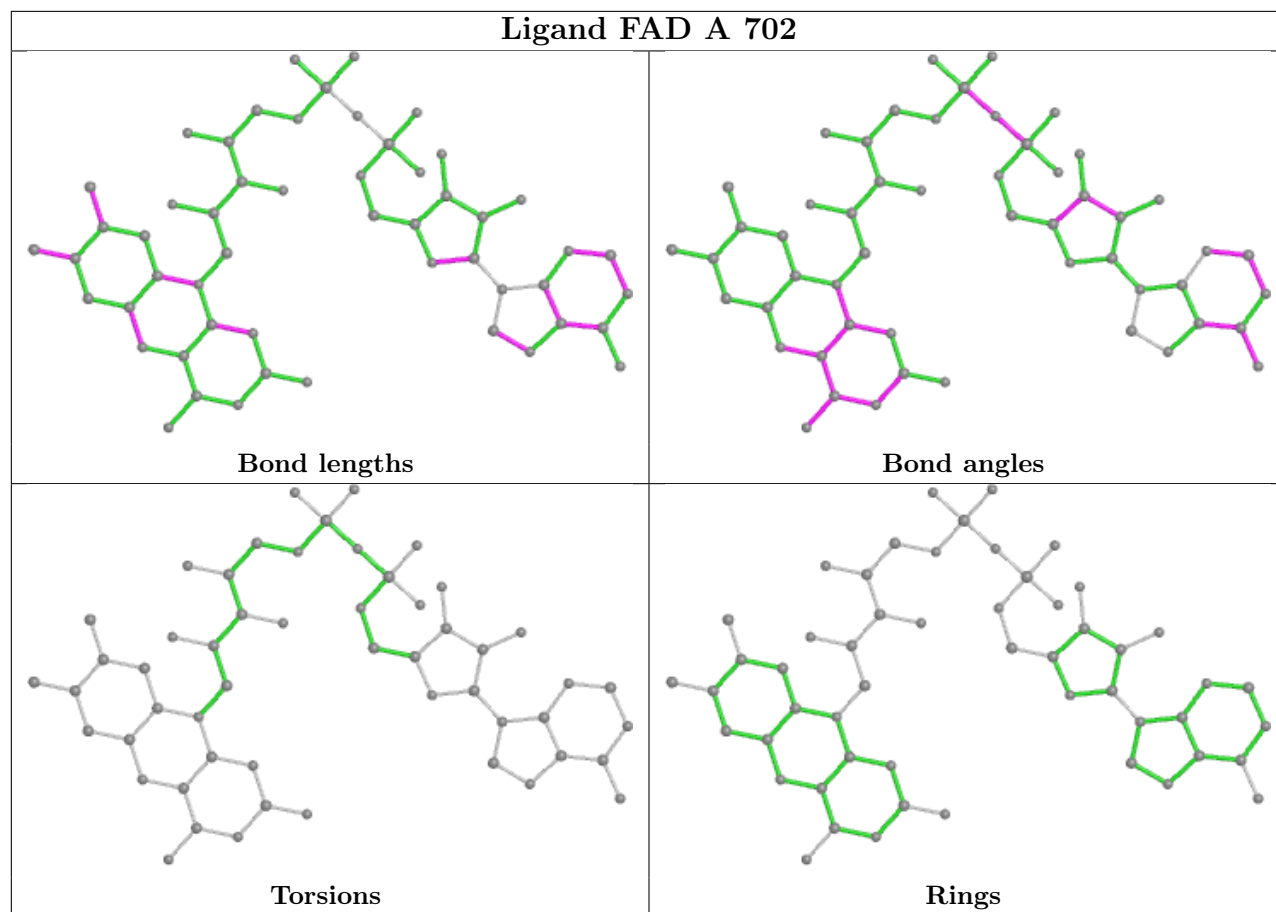
## Ligand 2AM A 703



## Ligand FAD B 702







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	611/622 (98%)	-0.42	2 (0%) 94 95	19, 34, 54, 71	0
1	B	603/622 (96%)	0.06	29 (4%) 30 28	16, 43, 98, 103	0
All	All	1214/1244 (97%)	-0.18	31 (2%) 56 57	16, 36, 94, 103	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	ILE	5.0
1	B	192	LEU	3.9
1	B	135	PHE	3.7
1	B	125	LEU	3.6
1	B	227	VAL	3.5
1	B	134	VAL	3.3
1	B	198	GLN	3.3
1	B	168	PHE	3.1
1	B	163	LEU	3.1
1	A	633	ALA	3.0
1	B	228	CYS	2.9
1	B	187	TYR	2.8
1	B	123	SER	2.8
1	B	191	ARG	2.7
1	B	119	LEU	2.7
1	B	153	TYR	2.7
1	B	201	PHE	2.6
1	B	166	VAL	2.5
1	B	169	ALA	2.4
1	B	164	THR	2.3
1	B	162	ASP	2.3
1	B	231	PHE	2.2
1	A	345	ILE	2.2
1	B	180	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	103	HIS	2.1
1	B	205	LEU	2.1
1	B	181	PHE	2.1
1	B	67	SER	2.0
1	B	152	PHE	2.0
1	B	217	ILE	2.0
1	B	633	ALA	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

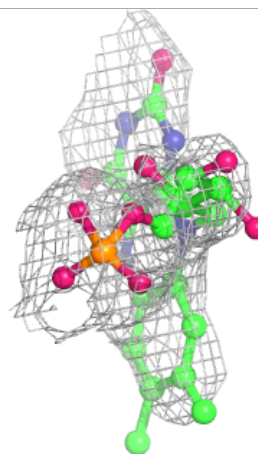
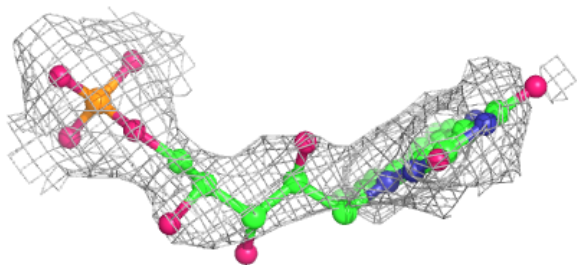
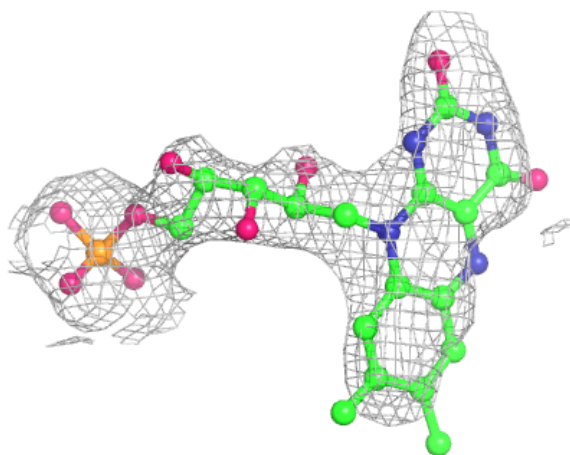
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	A	704	5/5	0.72	0.36	148,148,149,149	0
2	FMN	B	701	31/31	0.87	0.24	64,82,86,87	0
5	PO4	B	704	5/5	0.94	0.19	72,73,74,75	0
2	FMN	A	701	31/31	0.95	0.18	37,45,51,52	0
4	2AM	A	703	23/23	0.96	0.15	35,39,41,42	0
4	2AM	B	703	23/23	0.97	0.12	29,34,41,41	0
3	FAD	B	702	53/53	0.97	0.15	11,21,30,32	0
3	FAD	A	702	53/53	0.97	0.14	23,28,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around FMN B 701:**

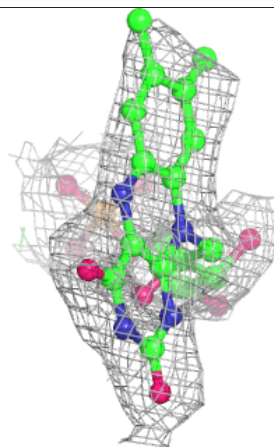
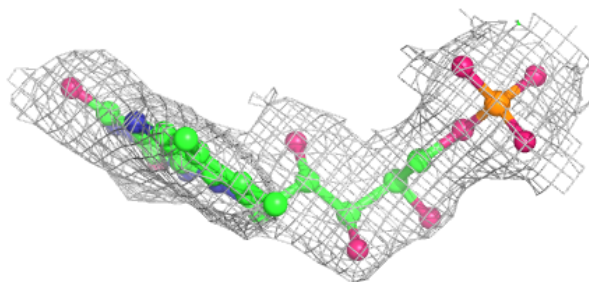
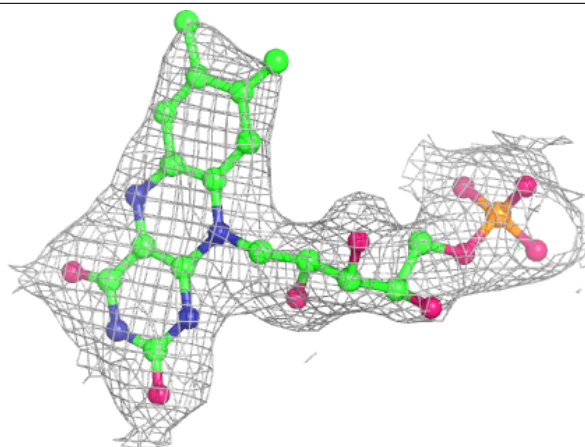
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





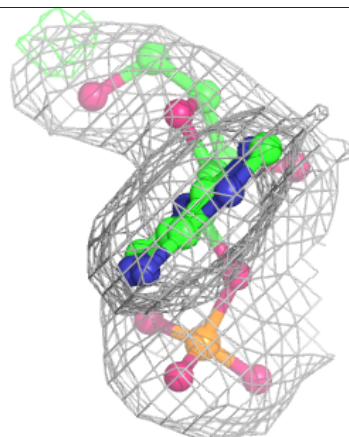
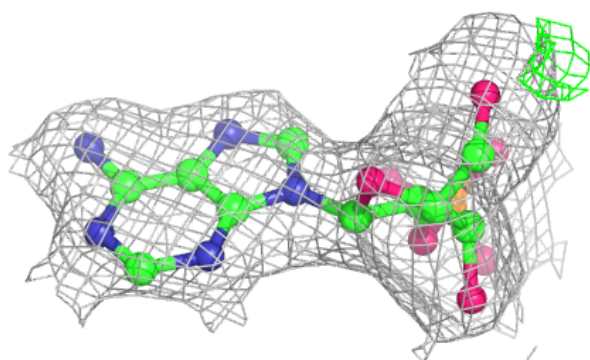
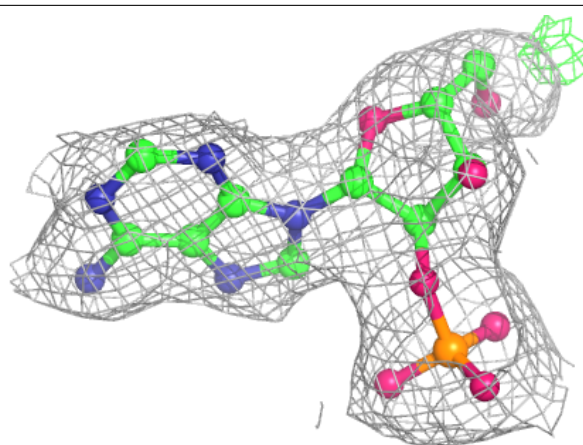
**Electron density around FMN A 701:**

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



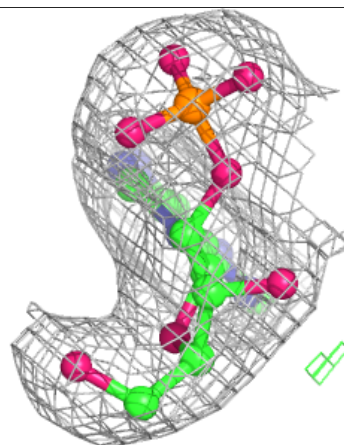
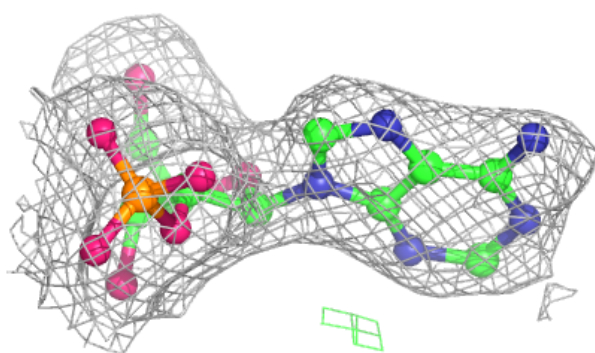
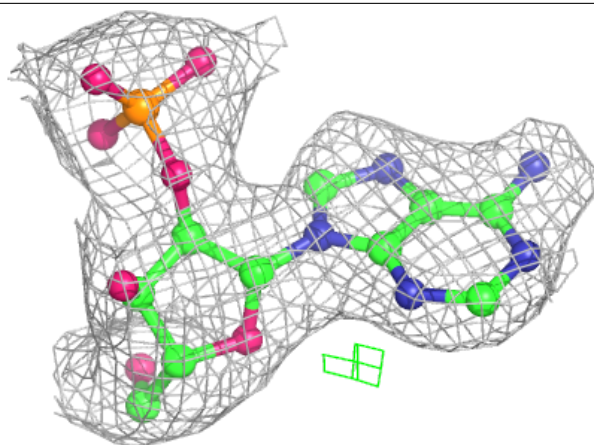
**Electron density around 2AM A 703:**

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

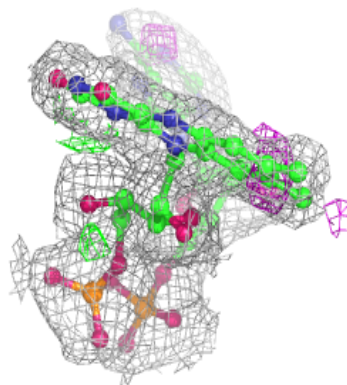
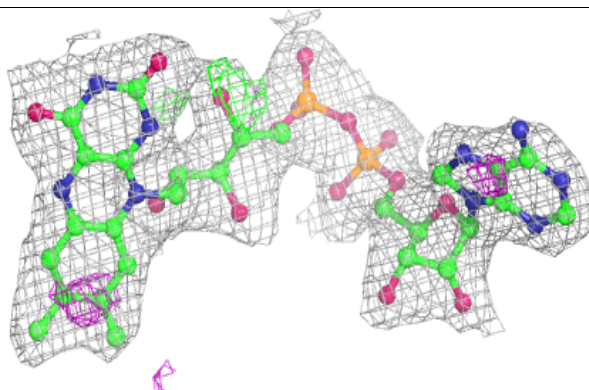
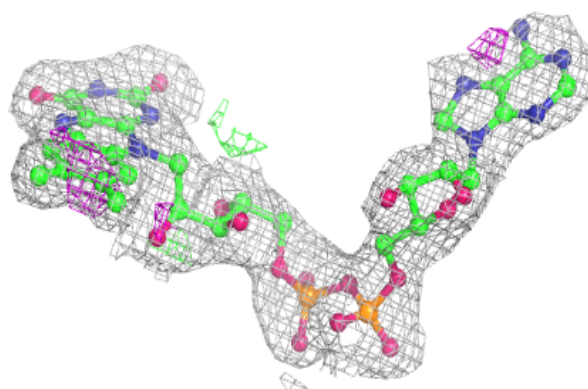


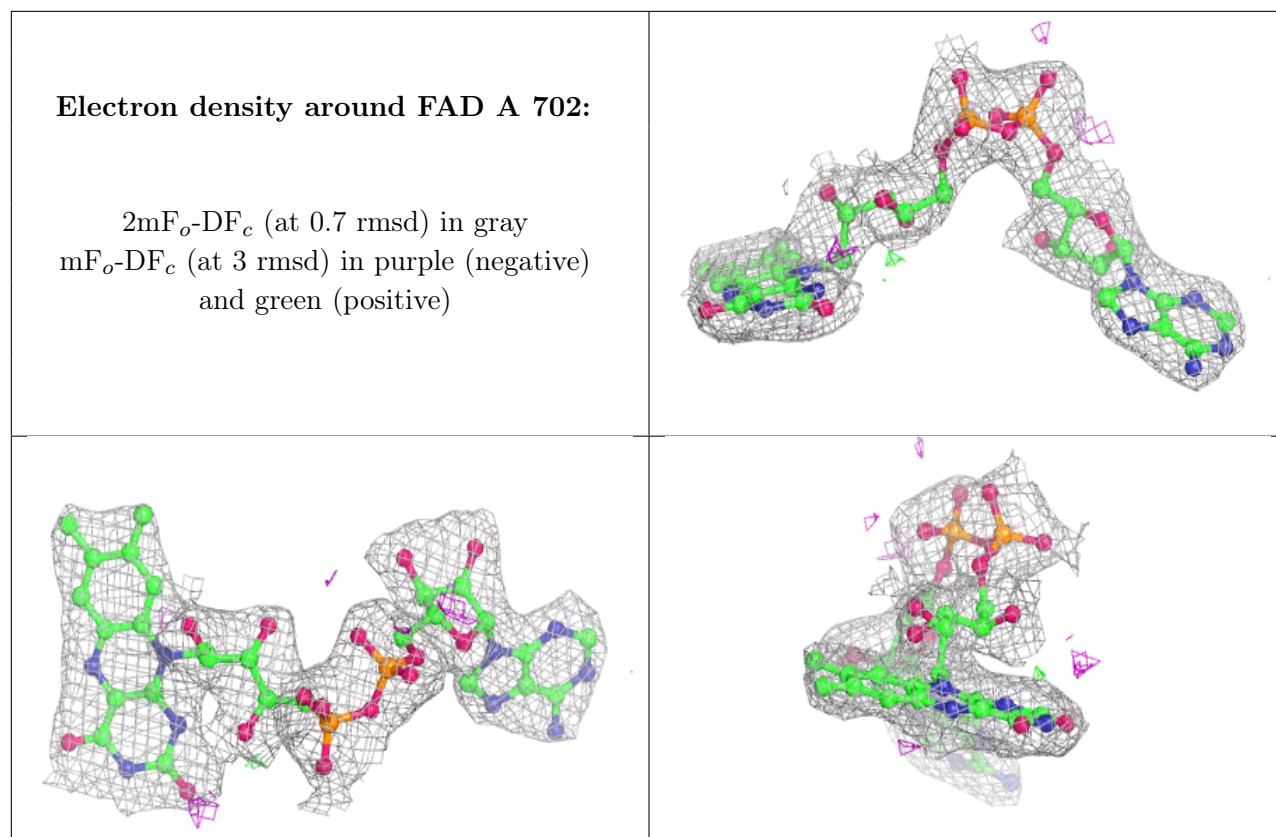
**Electron density around 2AM B 703:**

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

**Electron density around FAD B 702:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.