Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 04:48 am BST

PDB ID	:	4D7E
Title	:	An unprecedented NADPH domain conformation in Lysine Monooxygenase NbtG from Nocardia farcinica
Authors	:	Binda, C.; Robinson, R.; Keul, N.; Rodriguez, P.; Robinson, H.H.; Mattevi, A.; Sobrado, P.
Deposited on	:	2014-11-24
Resolution	:	2.40 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

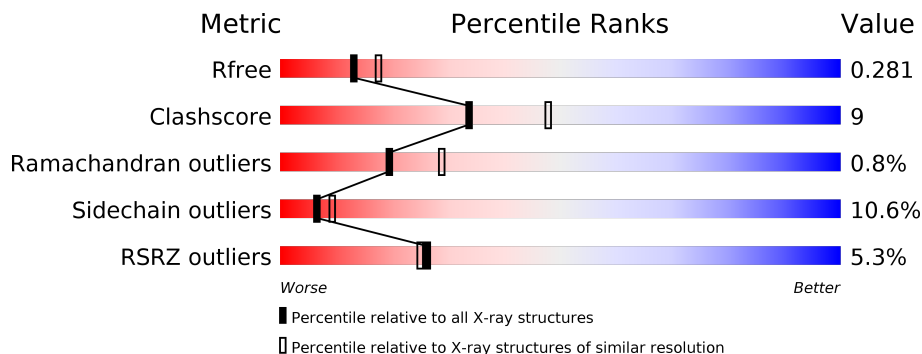|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
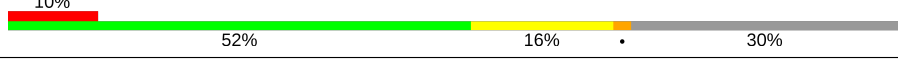*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.281
Clashscore		9
Ramachandran outliers		0.8%
Sidechain outliers		10.6%
RSRZ outliers		5.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	429	3% 68% 20% • 8%
1	B	429	2% 73% 16% • 9%
1	C	429	4% 68% 17% • 12%
1	D	429	10% 52% 16% • 30%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11714 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 L-LYS MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3045	1921	555	560	9			
1	B	392	Total	C	N	O	S	0	0	0
			3005	1899	544	556	6			
1	C	377	Total	C	N	O	S	0	0	0
			2885	1824	521	534	6			
1	D	300	Total	C	N	O	S	0	0	0
			2329	1482	412	430	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ALA	LYS	engineered mutation	UNP Q5Z1T5
B	184	ALA	LYS	engineered mutation	UNP Q5Z1T5
C	184	ALA	LYS	engineered mutation	UNP Q5Z1T5
D	184	ALA	LYS	engineered mutation	UNP Q5Z1T5

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

FAD

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

- Molecule 3 is water.

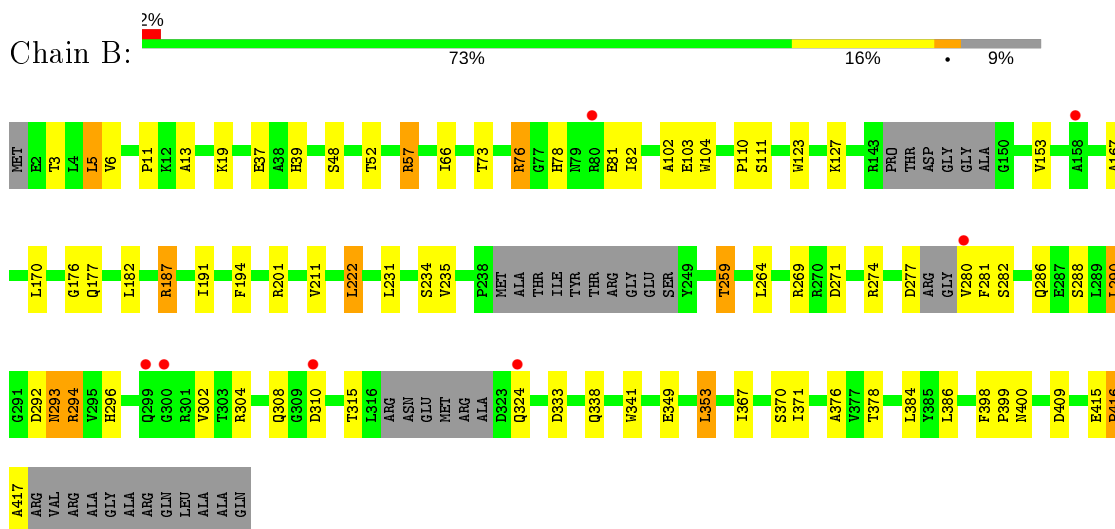| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	69	Total	O	0	0
			69	69		
3	C	52	Total	O	0	0
			52	52		
3	D	49	Total	O	0	0
			49	49		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: L-LYS MONOOXYGENASE

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MET E2 T3 V6 A13 L26 S29 I34 E37 N44 W45 L46 A47 W51 E63 K64 D65 I66 S72 T73 W74 A75 R76 N79 M87 W91 T92 S93 F94 W104 R107 P110 Y120 K127 L134 G135 R138 T139 Q142

ARG PRO THR ASP GLY ALA G150 E154 V155 A156 G157 A158 ASP G160 A161 T162 T163 P175 L182 R187 V188 L189 L197 R201 K202 L203 P204 I205 S206 S207 R208 V211 L222 R227 M230 S237 P238 MET ALA THR ILE TYR THR ARG GLY GLU SER Y249

F250 E251 N252 S253 L254 P258 W261 L264 Q267 E268 R269 R270 D271 V272 ILE ARG ARG THR ASP ARG GLY VAL PHE SER VAL ARG VAL Q286 L290 Q299 D310 L316 R317 N318 GLU MET ARG ALA D323 Q324 V325 R326 N327 L330 V331 V332 D333 Q338 P339 L340

D347 S348 E349 S350 L353 V358 Q364 Q365 R366 S369 S370 I371 L386 M389 G395 F398 P399 L407 L412 R413 ALA GLU PRO ALA ARG VAL ARG GLY ALA ARG GLN LEU ALA ALA GLN

● **Molecule 1: L-LYS MONOOXYGENASE**

Chain D:

10%

52%   16%   30%

MET E2 P11 R24 G27 L28 A40 W51 T52 D53 G54 R55 K64 F68 P69 W74 A75 R76 G77 H78 N79 R80 E81 S93 F94 L95 V96 E97 E103 R107 S111 H115 V116 W117 A118 K119 Y120 W123 K127 I128 D129 L134 V137

R138 T139 I140 R141 Q142 ARG PRO THR ASP GLY GLY ALA G150 V153 E154 G157 ALA ASP GLY ALA T162 T163 A167 D168 G169 L170 G176 K180 A181 LEU ALA ALA HIS PRO ARG VAL L189 S190 I191 A192 E193 F194 L197 ALA GLY LYS ARG LYS LEU PRO ILE SER SER ARG

ALA A210 V211 I212 G213 GLY GLY E216 T217 S220 A221 L222 D223 E224 L225 V226 R227 H228 GLU MET LEU THR ILE SER VAL ILE SER PRO MET ALA THR ILE TYR THR ARG ILE VAL GLY GLN GLY ASP GLY VAL ALA VAL THR LEU ARG ASN GLU MET ARG ALA ASP GLN VAL HIS ASN PHE ASP LEU VAL Y249 F250 E251 N252 S253 S256 D257 P258 T259 K260 W261 N262 A263 L264 S265 I266 Q267 E268 R269

V272 I273 R274 R275 T276 D277 ARG GLY VAL PHE SER VAL ARG VAL GLN GLU SER LEU LEU GLY ASP ASN ARG VAL HIS HIS LEU GLN GLY ARG VAL THR ARG ILE VAL GLY GLN GLY ASP GLY VAL ALA VAL THR LEU ARG ASN GLU MET ARG ALA ASP GLN VAL HIS ASN PHE ASP LEU VAL

VAL ASP ALA THR GLY GLY Q338 W341 S348 L354 E355 V358 P361 Q364 Q365 R366 S369 Y373 D374 L375 A376 V377 T378 G379 L380 G381 A382 K383 L384 Y385 L386 A390 A391 L392 N400 C403 E406 L407 R410 V411 L412 R413 ALA GLU PRO ALA ARG

VAL ARG ALA GLY ALA ARG GLN LEU ALA ALA GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.64Å 121.92Å 91.86Å 90.00° 97.72° 90.00°	Depositor
Resolution (Å)	91.19 – 2.40 45.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (91.19-2.40) 99.2 (45.51-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.208 , 0.281 0.210 , 0.281	Depositor DCC
R_{free} test set	2819 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.9	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11714	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.74	2/3109 (0.1%)	0.83	0/4217
1	B	0.69	0/3069	0.83	2/4167 (0.0%)
1	C	0.63	0/2946	0.80	1/3998 (0.0%)
1	D	0.62	1/2380 (0.0%)	0.74	0/3227
All	All	0.68	3/11504 (0.0%)	0.81	3/15609 (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	C	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	390	ALA	C-O	6.33	1.35	1.23
1	A	111	SER	CB-OG	6.27	1.50	1.42
1	A	104	TRP	CE3-CZ3	5.20	1.47	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	57	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	294	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	ASP	Peptide
1	C	2	GLU	Peptide
1	D	390	ALA	Mainchain

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	3045	0	3031	56	0
1	B	3005	0	2979	44	1
1	C	2885	0	2855	42	1
1	D	2329	0	2287	49	0
2	A	53	0	31	2	0
2	B	53	0	31	6	0
2	C	53	0	31	2	0
2	D	53	0	31	6	0
3	A	68	0	0	5	0
3	B	69	0	0	6	1
3	C	52	0	0	0	1
3	D	49	0	0	10	0
All	All	11714	0	11276	194	2

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 9.

All (194) 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:273:ILE:O	1:A:276:THR:HG22	1.32	1.24
1:D:403:CYS:O	3:D:2031:HOH:O	1.79	0.98
1:D:364:GLN:OE1	3:D:2027:HOH:O	1.93	0.86
1:A:240:ALA:HA	1:A:297:HIS:CE1	2.14	0.81
1:D:180:LYS:O	1:D:338:GLN:NE2	2.15	0.79
1:B:73:THR:OG1	1:B:259:THR:HG21	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:HIS:HB2	3:B:2051:HOH:O	1.85	0.77
1:D:364:GLN:NE2	3:D:2027:HOH:O	2.18	0.74
1:D:384:LEU:CD2	1:D:386:LEU:HD21	2.17	0.74
1:D:220:SER:O	1:D:223:ASP:HB3	1.87	0.73
1:D:403:CYS:HB2	3:D:2031:HOH:O	1.88	0.71
1:A:273:ILE:O	1:A:276:THR:CG2	2.26	0.71
1:D:406:GLU:CB	3:D:2031:HOH:O	2.39	0.70
3:A:2024:HOH:O	1:C:92:THR:HG23	1.91	0.70
1:A:199:GLY:HA3	3:A:2040:HOH:O	1.94	0.68
1:B:177:GLN:OE1	1:B:338:GLN:NE2	2.27	0.67
1:C:407:LEU:C	1:C:407:LEU:HD23	2.14	0.67
1:A:226:VAL:HG11	1:A:289:LEU:HD21	1.77	0.66
1:D:364:GLN:CD	3:D:2027:HOH:O	2.31	0.66
1:C:290:LEU:HD22	1:D:107:ARG:HA	1.78	0.65
1:D:365:GLN:O	1:D:369:SER:OG	2.15	0.63
1:D:103:GLU:O	1:D:107:ARG:HG3	1.99	0.62
1:D:406:GLU:O	1:D:410:ARG:HG2	1.98	0.62
1:B:280:VAL:HG13	1:B:281:PHE:H	1.65	0.62
1:D:24:ARG:HA	1:D:28:LEU:O	2.00	0.61
1:A:267:GLN:HB2	3:A:2049:HOH:O	1.99	0.61
1:B:293:ASN:HD22	1:B:293:ASN:H	1.46	0.60
1:C:250:PHE:O	1:C:254:LEU:HG	2.00	0.60
1:D:220:SER:O	1:D:223:ASP:CB	2.50	0.59
1:B:123:TRP:CZ2	1:B:127:LYS:HD2	2.37	0.59
1:A:189:LEU:HD22	1:A:330:LEU:HD11	1.83	0.59
1:C:6:VAL:HG11	1:C:13:ALA:HB2	1.85	0.59
1:D:40:ALA:HB1	3:D:2004:HOH:O	2.03	0.58
1:A:123:TRP:CZ2	1:A:127:LYS:HD2	2.39	0.58
1:D:140:ILE:HG12	1:D:153:VAL:HG23	1.85	0.58
1:B:187:ARG:NE	1:B:310:ASP:O	2.38	0.57
1:C:211:VAL:HG21	1:C:222:LEU:HD13	1.86	0.57
2:B:500:FAD:O4'	2:B:500:FAD:O2'	2.11	0.56
1:A:240:ALA:CA	1:A:297:HIS:CE1	2.86	0.56
1:C:237:SER:O	1:C:299:GLN:HA	2.05	0.56
1:B:292:ASP:OD1	1:B:294:ARG:HD3	2.06	0.56
1:D:376:ALA:HB2	1:D:385:TYR:CE1	2.41	0.56
1:A:371:ILE:HD13	1:A:389:MET:HB2	1.87	0.56
1:B:37:GLU:OE2	2:B:500:FAD:O2B	2.22	0.56
1:B:282:SER:O	1:B:286:GLN:HB2	2.06	0.55
1:C:91:TRP:O	1:C:94:PHE:HB3	2.06	0.55
1:A:283:VAL:O	1:A:287:GLU:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASN:N	1:A:262:ASN:OD1	2.39	0.55
1:D:373:TYR:CZ	1:D:410:ARG:NH1	2.75	0.55
1:A:391:ALA:HA	1:A:395:GLY:O	2.07	0.55
1:B:191:ILE:O	1:B:194:PHE:HB3	2.08	0.54
1:D:220:SER:O	1:D:223:ASP:N	2.41	0.54
1:B:176:GLY:HA2	1:B:341:TRP:CG	2.43	0.54
1:C:412:LEU:O	1:C:413:ARG:HB3	2.08	0.54
1:A:226:VAL:HG11	1:A:289:LEU:CD2	2.37	0.54
1:D:117:TRP:O	1:D:120:TYR:HB3	2.08	0.53
1:D:273:ILE:O	1:D:276:THR:HG22	2.09	0.53
1:D:261:TRP:CE2	1:D:269:ARG:HD2	2.43	0.53
1:D:407:LEU:HD23	1:D:407:LEU:C	2.29	0.53
1:B:211:VAL:HG21	1:B:222:LEU:HD13	1.90	0.53
1:D:150:GLY:N	1:D:382:ALA:HB2	2.24	0.52
1:D:256:SER:HA	1:D:403:CYS:HB3	1.90	0.52
1:A:74:TRP:O	1:A:76:ARG:N	2.42	0.52
1:D:358:VAL:CG1	1:D:366:ARG:HG2	2.40	0.52
1:B:73:THR:OG1	1:B:259:THR:CG2	2.56	0.52
1:B:123:TRP:CZ2	1:B:127:LYS:CD	2.93	0.51
1:A:200:LYS:O	1:A:201:ARG:C	2.48	0.51
1:A:239:MET:HE1	1:A:274:ARG:HB3	1.92	0.51
1:B:5:LEU:HD12	1:B:167:ALA:HB2	1.92	0.51
1:D:361:PRO:O	1:D:366:ARG:HD2	2.10	0.51
1:B:400:ASN:HA	2:B:500:FAD:O3'	2.10	0.51
1:A:216:GLU:HG2	1:A:278:ARG:CB	2.41	0.51
1:C:104:TRP:CD1	1:C:110:PRO:HD2	2.46	0.50
1:A:273:ILE:C	1:A:276:THR:HG22	2.22	0.50
1:A:216:GLU:HG2	1:A:278:ARG:HB2	1.93	0.50
1:B:367:ILE:O	1:B:371:ILE:CD1	2.60	0.50
1:B:416:PRO:O	1:B:417:ALA:HB2	2.12	0.50
1:C:251:GLU:HG3	1:C:252:ASN:H	1.76	0.50
1:C:330:LEU:C	1:C:330:LEU:HD23	2.33	0.49
1:D:384:LEU:HD23	1:D:386:LEU:HD21	1.94	0.49
1:B:293:ASN:ND2	1:B:293:ASN:H	2.11	0.49
1:A:197:LEU:CD1	1:A:203:LEU:HD23	2.43	0.49
1:D:68:PHE:HB3	3:D:2008:HOH:O	2.13	0.49
1:D:384:LEU:HD21	1:D:386:LEU:HD21	1.91	0.49
1:D:68:PHE:CD1	1:D:69:PRO:HA	2.48	0.49
1:A:251:GLU:OE2	1:A:275:ARG:NH1	2.44	0.48
1:A:371:ILE:CD1	1:A:389:MET:HB2	2.43	0.48
1:A:398:PHE:N	1:A:399:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:TRP:CE2	1:C:269:ARG:HG2	2.49	0.48
2:D:500:FAD:O2'	2:D:500:FAD:H9	2.14	0.48
1:A:218:ALA:HA	1:A:334:ALA:HB1	1.96	0.48
1:C:371:ILE:HD13	1:C:389:MET:O	2.14	0.48
1:D:78:HIS:HB3	1:D:81:GLU:HG2	1.96	0.48
2:B:500:FAD:H5'1	3:B:2003:HOH:O	2.12	0.48
1:B:19:LYS:NZ	3:B:2005:HOH:O	2.47	0.48
1:B:6:VAL:HG11	1:B:13:ALA:HB2	1.96	0.48
1:A:201:ARG:NH1	1:B:201:ARG:HB2	2.29	0.48
1:B:39:HIS:NE2	1:B:48:SER:OG	2.42	0.48
2:D:500:FAD:C2'	2:D:500:FAD:C9	2.91	0.48
1:D:64:LYS:HG2	1:D:68:PHE:CE2	2.48	0.47
1:A:47:ALA:HB2	1:A:53:ASP:O	2.14	0.47
1:A:255:PHE:HB3	1:A:402:SER:HB3	1.95	0.47
1:A:65:ASP:HB2	1:A:120:TYR:OH	2.15	0.47
2:A:500:FAD:O3'	2:A:500:FAD:N1	2.44	0.47
1:B:104:TRP:CD1	1:B:110:PRO:HD2	2.50	0.47
1:C:347:ASP:OD1	1:C:350:SER:OG	2.33	0.47
1:A:407:LEU:HD23	1:A:407:LEU:C	2.35	0.47
1:C:3:THR:HG23	1:C:34:ILE:HD12	1.96	0.47
1:A:104:TRP:CD1	1:A:110:PRO:HD2	2.50	0.47
1:A:133:VAL:HG21	1:A:165:LEU:HD11	1.95	0.47
1:D:170:LEU:HD23	1:D:384:LEU:HD12	1.97	0.47
1:D:273:ILE:O	1:D:276:THR:CG2	2.63	0.47
1:A:289:LEU:HD22	1:A:295:VAL:HG21	1.96	0.47
1:D:264:LEU:CD1	1:D:269:ARG:HG2	2.43	0.47
1:C:227:ARG:NE	1:D:227:ARG:NH2	2.63	0.46
1:A:290:LEU:O	1:B:57:ARG:NH2	2.40	0.46
1:C:358:VAL:HG13	1:C:366:ARG:HG2	1.97	0.46
1:C:339:PRO:HB3	1:C:389:MET:HE2	1.98	0.46
1:A:216:GLU:OE2	1:A:278:ARG:HB3	2.16	0.46
1:C:197:LEU:HD21	1:C:202:LYS:O	2.16	0.46
1:A:297:HIS:CE1	1:A:298:LEU:O	2.69	0.46
1:C:197:LEU:HD22	1:C:203:LEU:HD22	1.97	0.46
1:C:44:ASN:ND2	2:C:500:FAD:O1A	2.48	0.46
1:D:11:PRO:HD2	2:D:500:FAD:O2A	2.16	0.46
1:C:37:GLU:O	1:C:135:GLY:N	2.48	0.45
2:C:500:FAD:N1	2:C:500:FAD:O3'	2.49	0.45
3:A:2024:HOH:O	1:C:92:THR:CG2	2.58	0.45
1:A:199:GLY:O	1:B:201:ARG:CZ	2.65	0.45
1:A:373:TYR:O	1:A:410:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:HD12	1:C:230:MET:CE	2.46	0.45
1:A:96:VAL:HG21	1:C:87:MET:SD	2.56	0.45
1:D:400:ASN:HB2	2:D:500:FAD:N1	2.31	0.45
1:A:281:PHE:HB3	1:A:286:GLN:HG3	1.99	0.45
1:C:333:ASP:OD1	1:C:333:ASP:C	2.55	0.45
1:D:194:PHE:CE1	1:D:221:ALA:HB1	2.52	0.45
1:B:349:GLU:O	1:B:353:LEU:HB2	2.16	0.45
1:C:203:LEU:HD12	1:C:230:MET:HE1	1.98	0.45
1:D:406:GLU:HB2	3:D:2031:HOH:O	2.09	0.45
2:D:500:FAD:C2'	2:D:500:FAD:H9	2.47	0.45
1:A:73:THR:HG21	1:A:259:THR:HG21	1.99	0.45
1:A:113:GLN:OE1	1:A:115:HIS:NE2	2.50	0.44
1:A:384:LEU:HG	1:A:386:LEU:HD13	1.99	0.44
1:A:262:ASN:C	1:A:264:LEU:H	2.20	0.44
1:D:406:GLU:HB3	3:D:2031:HOH:O	2.09	0.44
1:C:46:LEU:O	1:C:47:ALA:C	2.55	0.44
1:C:74:TRP:HB2	1:C:79:ASN:OD1	2.18	0.44
2:A:500:FAD:H5'1	3:A:2003:HOH:O	2.18	0.44
1:D:123:TRP:CZ2	1:D:127:LYS:HD2	2.52	0.44
1:A:141:ARG:HD2	1:A:347:ASP:OD2	2.17	0.44
1:B:222:LEU:HD21	1:B:235:VAL:HG13	2.00	0.44
1:D:176:GLY:HA2	1:D:341:TRP:CD2	2.53	0.44
1:A:141:ARG:HA	1:A:350:SER:OG	2.18	0.44
1:B:338:GLN:HG2	1:B:338:GLN:O	2.18	0.44
1:D:264:LEU:HD13	1:D:269:ARG:HG2	1.99	0.44
1:A:68:PHE:CG	1:A:69:PRO:HA	2.52	0.43
1:B:177:GLN:HG3	3:B:2042:HOH:O	2.17	0.43
1:A:187:ARG:HD2	1:A:329:ASP:O	2.18	0.43
1:A:263:ALA:C	1:A:264:LEU:HD12	2.38	0.43
2:B:500:FAD:O3'	2:B:500:FAD:N1	2.52	0.43
1:B:11:PRO:HD2	2:B:500:FAD:O2A	2.20	0.42
1:C:330:LEU:HD23	1:C:331:VAL:N	2.35	0.42
1:C:339:PRO:HB3	1:C:389:MET:CE	2.49	0.42
1:C:398:PHE:N	1:C:399:PRO:CD	2.82	0.42
1:D:115:HIS:O	1:D:118:ALA:HB3	2.20	0.42
1:C:267:GLN:O	1:C:268:GLU:C	2.55	0.42
1:D:358:VAL:HG12	1:D:366:ARG:HG2	2.01	0.42
1:A:101:TYR:OH	1:C:63:GLU:HB3	2.20	0.42
1:A:123:TRP:CZ2	1:A:127:LYS:CD	3.03	0.42
1:B:19:LYS:CE	1:B:409:ASP:OD1	2.68	0.42
1:B:5:LEU:O	1:B:170:LEU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:HIS:ND1	1:B:81:GLU:OE1	2.52	0.42
1:C:51:TRP:CZ2	1:C:175:PRO:HG2	2.55	0.41
1:A:276:THR:O	1:A:277:ASP:C	2.58	0.41
1:B:102:ALA:HB3	3:B:2029:HOH:O	2.20	0.41
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.93	0.41
1:C:340:LEU:HD21	1:C:364:GLN:HG3	2.02	0.41
1:B:264:LEU:O	1:B:269:ARG:HD2	2.20	0.41
1:C:261:TRP:CD1	1:C:395:GLY:HA2	2.56	0.41
1:C:65:ASP:HB2	1:C:120:TYR:OH	2.19	0.41
1:A:266:ILE:O	1:A:270:ARG:HB2	2.21	0.41
1:C:264:LEU:O	1:C:269:ARG:HD2	2.20	0.41
1:C:407:LEU:C	1:C:407:LEU:CD2	2.87	0.41
1:B:6:VAL:HG11	1:B:13:ALA:CB	2.50	0.41
2:D:500:FAD:O4'	2:D:500:FAD:O2'	2.25	0.41
1:B:103:GLU:N	3:B:2029:HOH:O	2.43	0.41
1:A:1:MET:HE1	1:A:169:GLY:HA3	2.03	0.41
1:A:32:ARG:NH2	1:A:131:GLU:OE2	2.54	0.41
1:A:197:LEU:HB2	1:A:202:LYS:HB2	2.02	0.40
1:B:304:ARG:HB3	1:B:315:THR:HB	2.03	0.40
1:B:398:PHE:N	1:B:399:PRO:CD	2.83	0.40
1:B:376:ALA:HA	1:B:384:LEU:O	2.21	0.40
1:D:137:VAL:HG13	1:D:153:VAL:CG2	2.50	0.40
1:B:333:ASP:C	1:B:333:ASP:OD1	2.60	0.40
1:C:258:PRO:O	1:C:261:TRP:HB3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2067:HOH:O	3:C:2025:HOH:O[2_646]	2.00	0.20
1:B:76:ARG:NH1	1:C:138:ARG:O[2_646]	2.05	0.15

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	388/429 (90%)	364 (94%)	21 (5%)	3 (1%)	19	29
1	B	382/429 (89%)	355 (93%)	23 (6%)	4 (1%)	15	23
1	C	365/429 (85%)	338 (93%)	24 (7%)	3 (1%)	19	29
1	D	284/429 (66%)	261 (92%)	21 (7%)	2 (1%)	22	32
All	All	1419/1716 (83%)	1318 (93%)	89 (6%)	12 (1%)	19	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ARG
1	A	319	GLU
1	C	201	ARG
1	D	220	SER
1	A	263	ALA
1	B	259	THR
1	B	302	VAL
1	C	74	TRP
1	C	251	GLU
1	B	415	GLU
1	D	258	PRO
1	B	416	PRO

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	316/336 (94%)	278 (88%)	38 (12%)	5	6
1	B	311/336 (93%)	286 (92%)	25 (8%)	12	18
1	C	298/336 (89%)	264 (89%)	34 (11%)	5	7
1	D	240/336 (71%)	214 (89%)	26 (11%)	6	9
All	All	1165/1344 (87%)	1042 (89%)	123 (11%)	6	9

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	LEU
1	A	5	LEU
1	A	24	ARG
1	A	26	LEU
1	A	55	ARG
1	A	111	SER
1	A	129	ASP
1	A	132	LEU
1	A	134	LEU
1	A	138	ARG
1	A	141	ARG
1	A	163	THR
1	A	164	GLU
1	A	205	ILE
1	A	208	ARG
1	A	229	GLU
1	A	231	LEU
1	A	248	SER
1	A	259	THR
1	A	262	ASN
1	A	266	ILE
1	A	267	GLN
1	A	276	THR
1	A	278	ARG
1	A	286	GLN
1	A	290	LEU
1	A	298	LEU
1	A	304	ARG
1	A	312	VAL
1	A	319	GLU
1	A	321	ARG
1	A	324	GLN
1	A	348	SER
1	A	349	GLU
1	A	356	LEU
1	A	364	GLN
1	A	386	LEU
1	B	3	THR
1	B	5	LEU
1	B	52	THR
1	B	66	ILE

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Mol	Chain	Res	Type
1	B	76	ARG
1	B	82	ILE
1	B	111	SER
1	B	153	VAL
1	B	182	LEU
1	B	187	ARG
1	B	222	LEU
1	B	231	LEU
1	B	234	SER
1	B	271	ASP
1	B	274	ARG
1	B	277	ASP
1	B	288	SER
1	B	290	LEU
1	B	293	ASN
1	B	308	GLN
1	B	324	GLN
1	B	353	LEU
1	B	370	SER
1	B	378	THR
1	B	386	LEU
1	C	2	GLU
1	C	26	LEU
1	C	29	SER
1	C	66	ILE
1	C	72	SER
1	C	92	THR
1	C	107	ARG
1	C	127	LYS
1	C	134	LEU
1	C	139	THR
1	C	154	GLU
1	C	162	THR
1	C	163	THR
1	C	182	LEU
1	C	187	ARG
1	C	189	LEU
1	C	203	LEU
1	C	222	LEU
1	C	227	ARG
1	C	250	PHE
1	C	253	SER

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Mol	Chain	Res	Type
1	C	264	LEU
1	C	270	ARG
1	C	271	ASP
1	C	290	LEU
1	C	327	ASN
1	C	338	GLN
1	C	349	GLU
1	C	350	SER
1	C	353	LEU
1	C	358	VAL
1	C	365	GLN
1	C	369	SER
1	C	386	LEU
1	D	52	THR
1	D	76	ARG
1	D	80	ARG
1	D	97	GLU
1	D	107	ARG
1	D	111	SER
1	D	119	LYS
1	D	129	ASP
1	D	134	LEU
1	D	139	THR
1	D	154	GLU
1	D	163	THR
1	D	197	LEU
1	D	253	SER
1	D	260	LYS
1	D	262	ASN
1	D	264	LEU
1	D	267	GLN
1	D	348	SER
1	D	355	GLU
1	D	364	GLN
1	D	366	ARG
1	D	369	SER
1	D	380	LEU
1	D	386	LEU
1	D	411	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	B	293	ASN
1	C	25	GLN
1	C	185	HIS
1	C	338	GLN
1	C	365	GLN
1	D	267	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	500	-	51,58,58	1.26	6 (11%)	60,89,89	2.77	21 (35%)
2	FAD	C	500	-	51,58,58	1.24	5 (9%)	60,89,89	2.24	19 (31%)
2	FAD	B	500	-	51,58,58	1.25	3 (5%)	60,89,89	2.66	22 (36%)
2	FAD	D	500	-	51,58,58	1.12	4 (7%)	60,89,89	1.91	15 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	500	-	-	11/30/50/50	0/6/6/6
2	FAD	C	500	-	-	15/30/50/50	0/6/6/6
2	FAD	B	500	-	-	11/30/50/50	0/6/6/6
2	FAD	D	500	-	-	10/30/50/50	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C9A-N10	4.86	1.45	1.38
2	A	500	FAD	C9A-N10	3.63	1.43	1.38
2	D	500	FAD	C9A-N10	3.46	1.43	1.38
2	C	500	FAD	C9A-N10	3.38	1.43	1.38
2	A	500	FAD	C1'-N10	3.38	1.51	1.48
2	C	500	FAD	O4B-C1B	3.36	1.45	1.41
2	B	500	FAD	C2'-C3'	-2.78	1.48	1.53
2	C	500	FAD	C5A-C4A	2.69	1.48	1.40
2	B	500	FAD	C5A-C4A	2.65	1.48	1.40
2	D	500	FAD	C5A-C4A	2.64	1.47	1.40
2	C	500	FAD	C9A-C5X	2.59	1.47	1.42
2	D	500	FAD	C10-N1	2.48	1.36	1.33
2	D	500	FAD	C9A-C5X	2.23	1.47	1.42
2	A	500	FAD	C9A-C5X	2.15	1.46	1.42
2	A	500	FAD	C2-N3	-2.08	1.34	1.38
2	A	500	FAD	O4B-C4B	-2.03	1.40	1.45
2	A	500	FAD	C4-N3	2.03	1.36	1.33
2	C	500	FAD	C2A-N3A	2.00	1.35	1.32

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	O4'-C4'-C5'	-9.70	88.13	109.92
2	B	500	FAD	O4'-C4'-C5'	-8.17	91.55	109.92
2	A	500	FAD	C5'-C4'-C3'	7.85	127.36	112.20
2	B	500	FAD	C5'-C4'-C3'	6.35	124.48	112.20
2	B	500	FAD	C4X-N5-C5X	6.18	122.95	116.77
2	A	500	FAD	O4'-C4'-C3'	-6.15	94.13	109.10
2	B	500	FAD	C4-N3-C2	6.11	120.30	115.14
2	A	500	FAD	C1'-N10-C9A	6.07	123.07	118.29
2	C	500	FAD	C4'-C3'-C2'	-5.44	102.06	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	FAD	C4X-N5-C5X	5.30	122.06	116.77
2	B	500	FAD	O4'-C4'-C3'	-5.26	96.30	109.10
2	D	500	FAD	C4X-N5-C5X	5.23	122.00	116.77
2	D	500	FAD	N3A-C2A-N1A	-5.06	120.77	128.68
2	D	500	FAD	C4'-C3'-C2'	-4.81	103.35	113.36
2	C	500	FAD	O4'-C4'-C5'	-4.81	99.10	109.92
2	C	500	FAD	C1'-N10-C10	4.77	122.68	118.41
2	A	500	FAD	C4'-C3'-C2'	-4.70	103.59	113.36
2	C	500	FAD	N3A-C2A-N1A	-4.61	121.47	128.68
2	C	500	FAD	C4-N3-C2	4.47	118.92	115.14
2	C	500	FAD	O3'-C3'-C4'	4.42	119.50	108.81
2	A	500	FAD	C9A-N10-C10	-4.40	116.15	121.91
2	B	500	FAD	C1B-N9A-C4A	-4.34	119.02	126.64
2	A	500	FAD	N3A-C2A-N1A	-4.31	121.94	128.68
2	D	500	FAD	C4-N3-C2	4.21	118.69	115.14
2	B	500	FAD	C4'-C3'-C2'	-4.15	104.74	113.36
2	B	500	FAD	N3A-C2A-N1A	-4.12	122.23	128.68
2	B	500	FAD	C1'-N10-C10	4.10	122.08	118.41
2	D	500	FAD	C4A-C5A-N7A	-4.06	105.17	109.40
2	A	500	FAD	O3'-C3'-C4'	3.92	118.27	108.81
2	C	500	FAD	O2'-C2'-C1'	3.91	119.01	109.59
2	A	500	FAD	O5'-C5'-C4'	3.76	119.41	109.36
2	A	500	FAD	C4A-C5A-N7A	-3.71	105.53	109.40
2	B	500	FAD	C2A-N1A-C6A	3.70	125.08	118.75
2	B	500	FAD	O3'-C3'-C4'	3.64	117.60	108.81
2	D	500	FAD	C1'-N10-C10	3.63	121.66	118.41
2	B	500	FAD	O2'-C2'-C1'	3.62	118.32	109.59
2	D	500	FAD	C2A-N1A-C6A	3.60	124.91	118.75
2	A	500	FAD	O4B-C1B-C2B	-3.47	101.85	106.93
2	C	500	FAD	C9A-N10-C10	-3.38	117.48	121.91
2	C	500	FAD	C6-C5X-N5	3.38	122.77	119.05
2	A	500	FAD	O3'-C3'-C2'	-3.33	100.77	108.81
2	B	500	FAD	C9A-N10-C10	-3.28	117.61	121.91
2	A	500	FAD	C4X-N5-C5X	3.26	120.03	116.77
2	B	500	FAD	C4X-C4-N3	-3.26	118.98	123.43
2	D	500	FAD	C1B-N9A-C4A	-3.18	121.06	126.64
2	C	500	FAD	C1B-N9A-C4A	-3.02	121.34	126.64
2	C	500	FAD	C4A-C5A-N7A	-3.01	106.26	109.40
2	C	500	FAD	C4X-C4-N3	-3.01	119.32	123.43
2	A	500	FAD	C4-C4X-C10	-2.92	118.02	119.95
2	A	500	FAD	C1B-N9A-C4A	-2.90	121.55	126.64
2	C	500	FAD	C5'-C4'-C3'	2.73	117.47	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	FAD	C4-N3-C2	2.64	117.37	115.14
2	C	500	FAD	C2B-C3B-C4B	2.64	107.77	102.64
2	A	500	FAD	C1'-N10-C10	2.60	120.74	118.41
2	B	500	FAD	O4B-C1B-C2B	-2.57	103.17	106.93
2	A	500	FAD	C2A-N1A-C6A	2.56	123.13	118.75
2	B	500	FAD	C1'-N10-C9A	2.54	120.29	118.29
2	B	500	FAD	O3'-C3'-C2'	-2.52	102.73	108.81
2	A	500	FAD	O2'-C2'-C1'	2.51	115.63	109.59
2	C	500	FAD	P-O3P-PA	-2.50	124.24	132.83
2	C	500	FAD	O3'-C3'-C2'	-2.48	102.82	108.81
2	D	500	FAD	C9A-C5X-N5	-2.43	118.57	122.36
2	A	500	FAD	P-O3P-PA	-2.42	124.52	132.83
2	D	500	FAD	C4X-C10-N10	-2.39	117.85	120.30
2	D	500	FAD	C6-C5X-N5	2.37	121.66	119.05
2	C	500	FAD	C2A-N1A-C6A	2.37	122.81	118.75
2	B	500	FAD	C4A-C5A-N7A	-2.36	106.94	109.40
2	B	500	FAD	O5B-PA-O1A	-2.29	100.12	109.07
2	D	500	FAD	C2B-C3B-C4B	2.29	107.08	102.64
2	A	500	FAD	C6-C5X-N5	2.26	121.54	119.05
2	B	500	FAD	C9A-C5X-N5	-2.23	118.87	122.36
2	B	500	FAD	O5'-P-O1P	2.22	117.75	109.07
2	D	500	FAD	C4X-C4-N3	-2.16	120.48	123.43
2	C	500	FAD	C9A-C5X-N5	-2.16	118.98	122.36
2	B	500	FAD	C9-C9A-C5X	-2.13	116.24	119.88
2	D	500	FAD	O2'-C2'-C1'	2.09	114.62	109.59
2	D	500	FAD	O3B-C3B-C2B	-2.01	105.31	111.82

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FAD	N10-C1'-C2'-O2'
2	A	500	FAD	N10-C1'-C2'-C3'
2	A	500	FAD	C3'-C4'-C5'-O5'
2	A	500	FAD	O4'-C4'-C5'-O5'
2	C	500	FAD	N10-C1'-C2'-O2'
2	C	500	FAD	N10-C1'-C2'-C3'
2	C	500	FAD	C2'-C3'-C4'-C5'
2	C	500	FAD	O3'-C3'-C4'-C5'
2	C	500	FAD	C3'-C4'-C5'-O5'
2	C	500	FAD	O4'-C4'-C5'-O5'
2	C	500	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	C	500	FAD	C5'-O5'-P-O3P
2	B	500	FAD	N10-C1'-C2'-O2'
2	B	500	FAD	N10-C1'-C2'-C3'
2	B	500	FAD	O3'-C3'-C4'-C5'
2	B	500	FAD	C3'-C4'-C5'-O5'
2	B	500	FAD	O4'-C4'-C5'-O5'
2	D	500	FAD	C2'-C1'-N10-C10
2	D	500	FAD	N10-C1'-C2'-O2'
2	D	500	FAD	N10-C1'-C2'-C3'
2	D	500	FAD	C5'-O5'-P-O2P
2	A	500	FAD	O3'-C3'-C4'-O4'
2	C	500	FAD	O3'-C3'-C4'-O4'
2	A	500	FAD	O3'-C3'-C4'-C5'
2	A	500	FAD	C2'-C3'-C4'-C5'
2	B	500	FAD	C2'-C3'-C4'-C5'
2	C	500	FAD	C2'-C3'-C4'-O4'
2	A	500	FAD	PA-O3P-P-O5'
2	C	500	FAD	PA-O3P-P-O5'
2	B	500	FAD	PA-O3P-P-O5'
2	D	500	FAD	PA-O3P-P-O5'
2	D	500	FAD	C5'-O5'-P-O3P
2	D	500	FAD	C5'-O5'-P-O1P
2	A	500	FAD	C1'-C2'-C3'-O3'
2	D	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	P-O3P-PA-O2A
2	D	500	FAD	P-O3P-PA-O2A
2	A	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	P-O3P-PA-O1A
2	B	500	FAD	P-O3P-PA-O1A
2	B	500	FAD	C5'-O5'-P-O1P
2	C	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	C1'-C2'-C3'-O3'
2	B	500	FAD	C1'-C2'-C3'-O3'
2	A	500	FAD	C2'-C3'-C4'-O4'
2	D	500	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	FAD	2	0
2	B	500	FAD	6	0
2	D	500	FAD	6	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 FAD A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 500

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 500

Bond lengths

Bond angles

Torsions

Rings
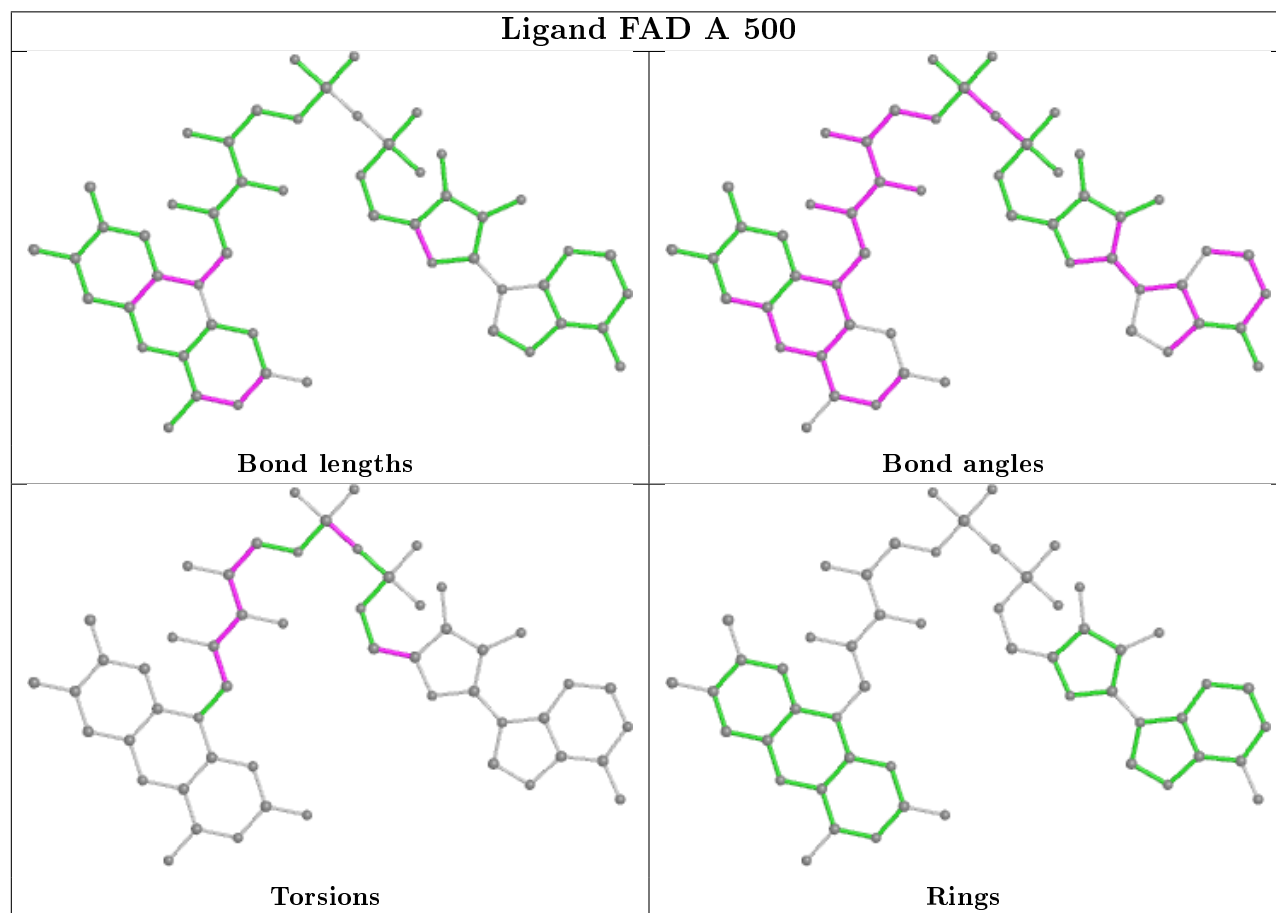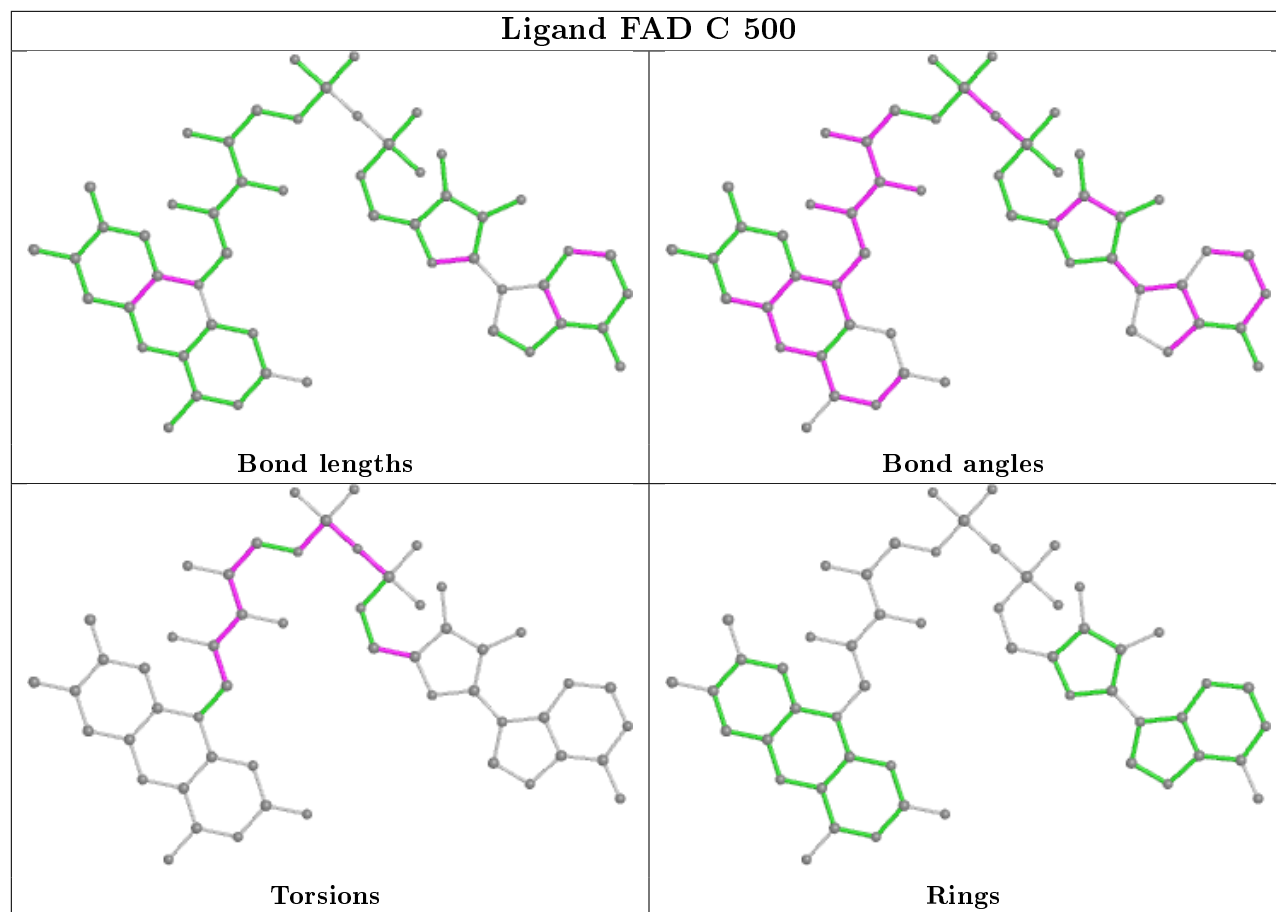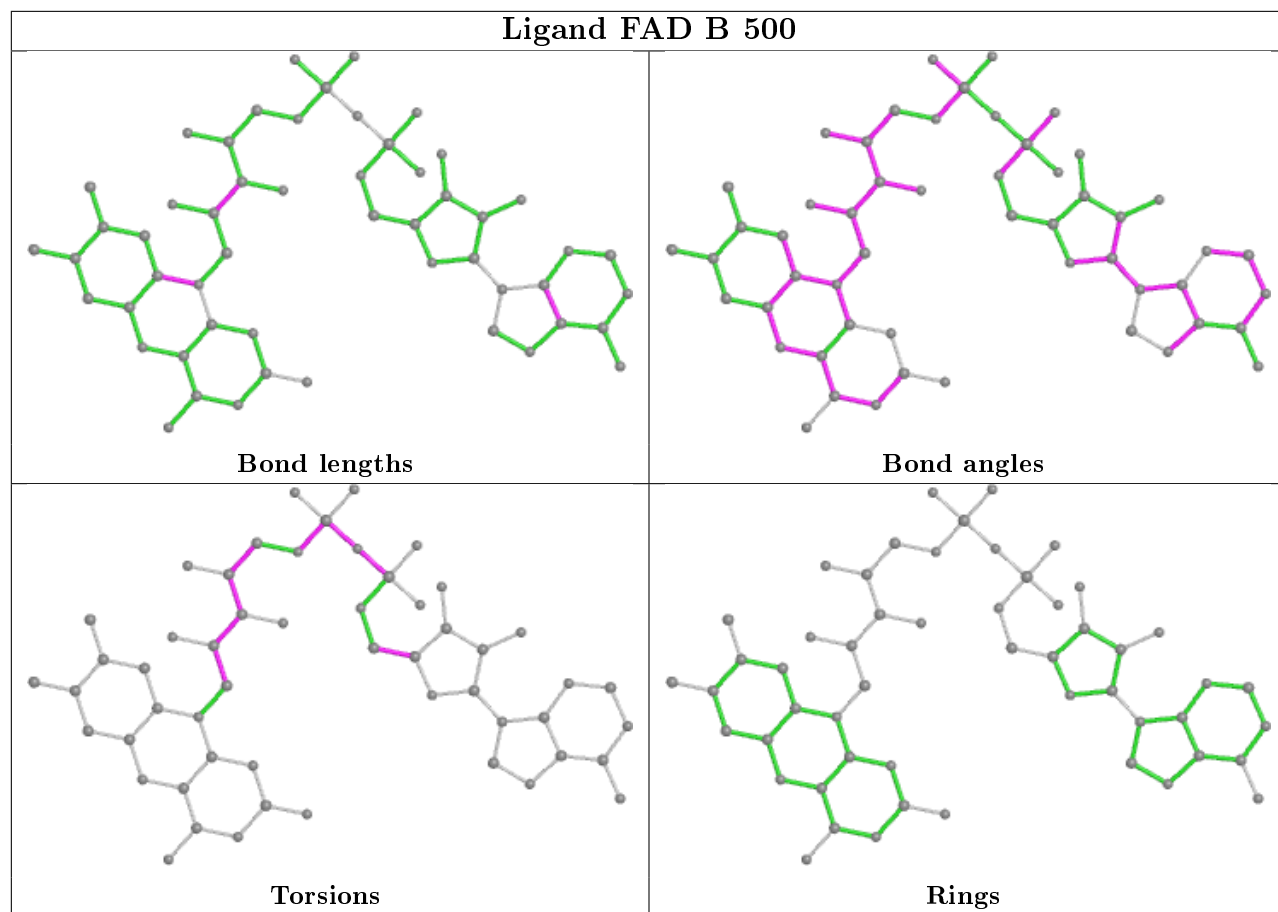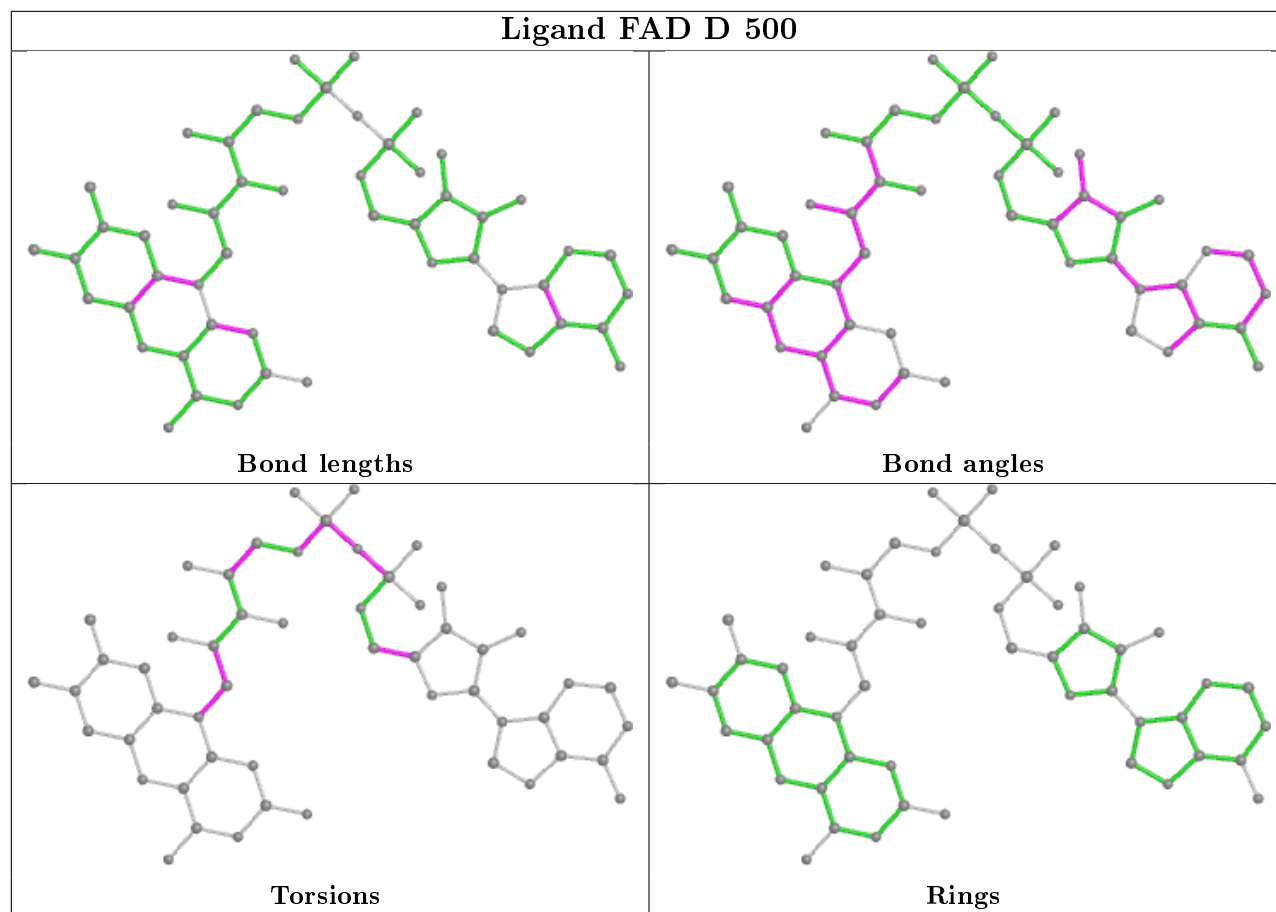
5.7 Other polymers (i)

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	396/429 (92%)	0.01	11 (2%)	53	51	36, 60, 99, 140	0
1	B	392/429 (91%)	0.05	7 (1%)	68	66	39, 63, 100, 126	0
1	C	377/429 (87%)	0.15	18 (4%)	30	29	37, 69, 111, 134	0
1	D	300/429 (69%)	0.63	41 (13%)	3	2	52, 85, 119, 145	0
All	All	1465/1716 (85%)	0.19	77 (5%)	26	25	36, 68, 111, 145	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	227	ARG	6.3
1	B	300	GLY	6.2
1	B	158	ALA	4.6
1	C	76	ARG	4.6
1	D	225	LEU	4.3
1	D	392	LEU	4.2
1	D	378	THR	4.2
1	D	275	ARG	4.1
1	D	221	ALA	3.9
1	D	55	ARG	3.9
1	D	74	TRP	3.6
1	D	54	GLY	3.6
1	D	354	LEU	3.6
1	C	250	PHE	3.4
1	D	27	GLY	3.4
1	C	324	GLN	3.3
1	D	191	ILE	3.3
1	D	379	GLY	3.2
1	C	163	THR	3.2
1	D	277	ASP	3.2
1	D	212	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	168	ASP	3.1
1	A	76	ARG	3.1
1	D	217	THR	3.0
1	D	211	VAL	3.0
1	D	226	VAL	3.0
1	C	318	ASN	3.0
1	A	162	THR	3.0
1	D	251	GLU	3.0
1	C	317	ARG	2.9
1	C	208	ARG	2.9
1	D	51	TRP	2.9
1	D	210	ALA	2.8
1	D	93	SER	2.8
1	D	272	VAL	2.8
1	D	266	ILE	2.7
1	C	325	VAL	2.7
1	D	263	ALA	2.7
1	A	319	GLU	2.7
1	D	228	HIS	2.7
1	A	320	MET	2.6
1	D	95	LEU	2.6
1	C	207	SER	2.6
1	B	280	VAL	2.6
1	C	161	ALA	2.6
1	A	281	PHE	2.6
1	D	194	PHE	2.6
1	D	181	ALA	2.5
1	D	262	ASN	2.5
1	D	381	GLY	2.5
1	C	205	ILE	2.5
1	C	74	TRP	2.4
1	C	310	ASP	2.4
1	A	163	THR	2.4
1	D	189	LEU	2.4
1	A	161	ALA	2.3
1	B	324	GLN	2.3
1	D	167	ALA	2.3
1	A	267	GLN	2.3
1	D	193	GLU	2.3
1	D	222	LEU	2.3
1	A	278	ARG	2.2
1	D	375	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	299	GLN	2.2
1	C	316	LEU	2.2
1	C	156	ALA	2.2
1	A	141	ARG	2.2
1	B	80	ARG	2.1
1	A	250	PHE	2.1
1	C	267	GLN	2.1
1	B	310	ASP	2.1
1	D	264	LEU	2.1
1	D	192	ALA	2.1
1	D	267	GLN	2.1
1	C	202	LYS	2.1
1	D	28	LEU	2.0
1	C	230	MET	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 carbohydrates 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	FAD	D	500	53/53	0.94	0.16	63,76,86,86	0
2	FAD	C	500	53/53	0.97	0.12	47,57,69,71	0
2	FAD	B	500	53/53	0.97	0.13	37,43,47,49	0
2	FAD	A	500	53/53	0.97	0.14	38,44,52,56	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 FAD D 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
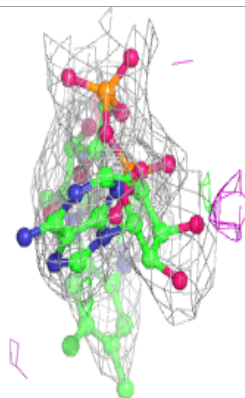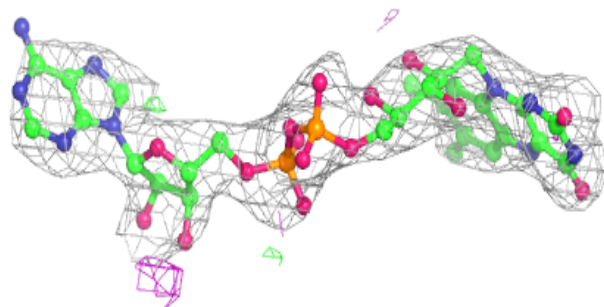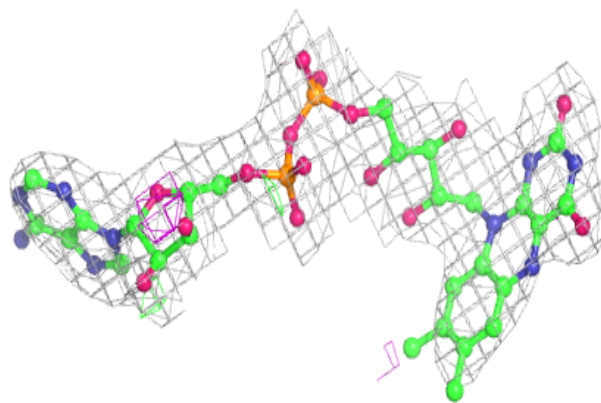
Electron density around FAD C 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
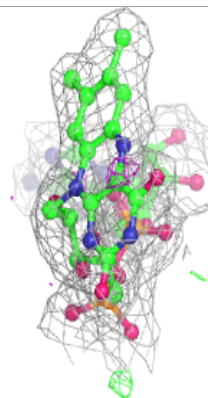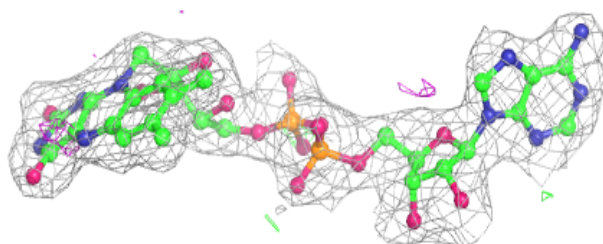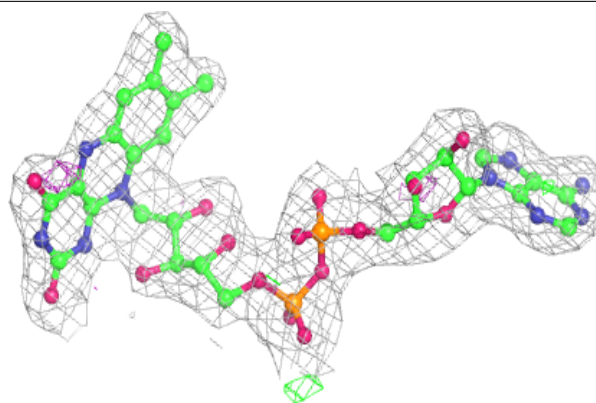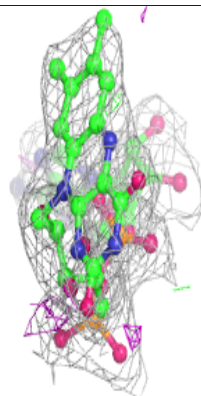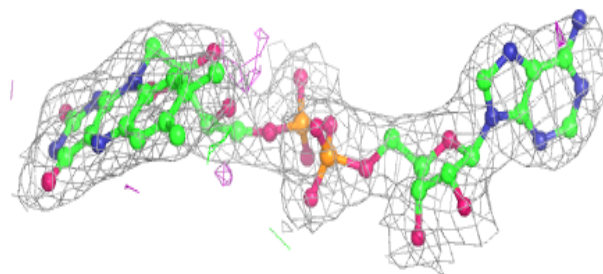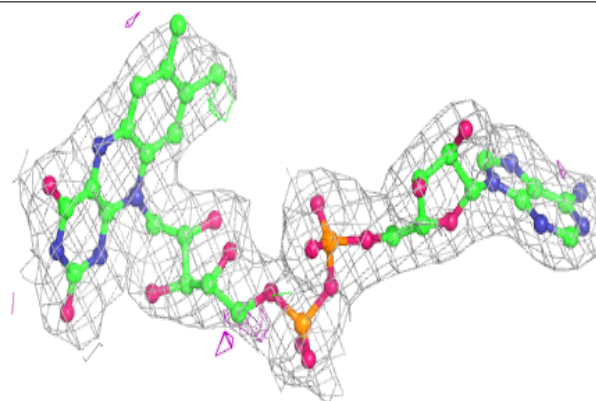$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
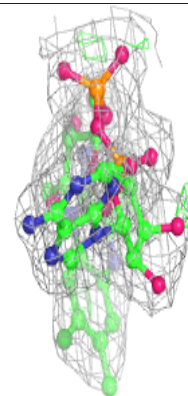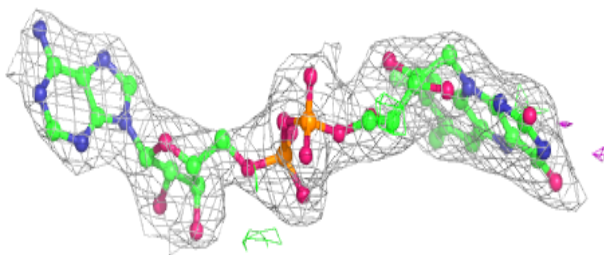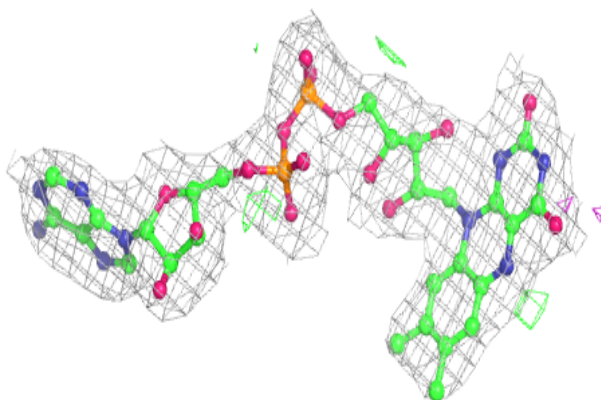
Electron density around FAD B 500:

$2mF_o$-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 500:

$2mF_o$-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.