Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 09:19 PM EST

PDB ID	:	3UKQ
Title	:	Crystal structure of R327K UDP-galactopyranose mutase from Aspergillus fumigatus in complex with UDPgalp
Authors	:	Van Straaten, K.E.; Sanders, D.A.R.
Deposited on	:	2011-11-09
Resolution	:	3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

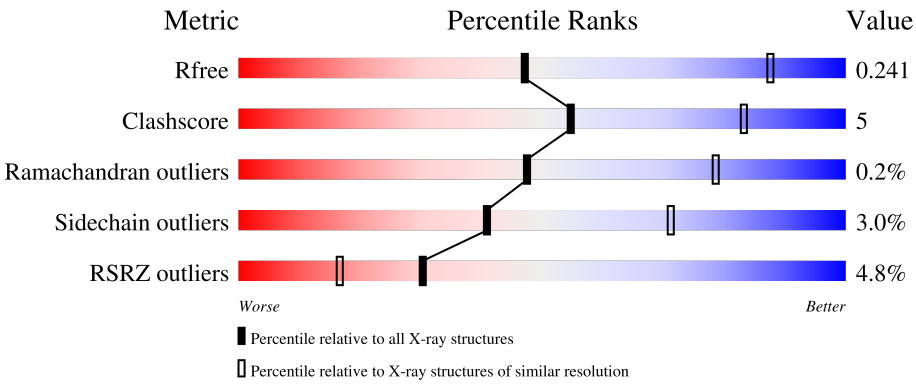
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	5% 87% 13%
1	B	510	4% 86% 13% •
1	C	510	4% 85% 15%
1	D	510	6% 84% 15% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16433 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 UDP-galactopyranose mutase.

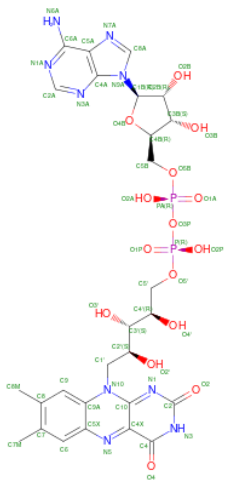
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	510	4002	2540	685	756	21	0	0	0
1	B	510	4002	2540	685	756	21	0	0	0
1	C	510	4002	2540	685	756	21	0	0	0
1	D	510	4002	2540	685	756	21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	LYS	ARG	engineered mutation	UNP Q4W1X2
A	511	LEU	-	expression tag	UNP Q4W1X2
B	327	LYS	ARG	engineered mutation	UNP Q4W1X2
B	511	LEU	-	expression tag	UNP Q4W1X2
C	327	LYS	ARG	engineered mutation	UNP Q4W1X2
C	511	LEU	-	expression tag	UNP Q4W1X2
D	327	LYS	ARG	engineered mutation	UNP Q4W1X2
D	511	LEU	-	expression tag	UNP Q4W1X2

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

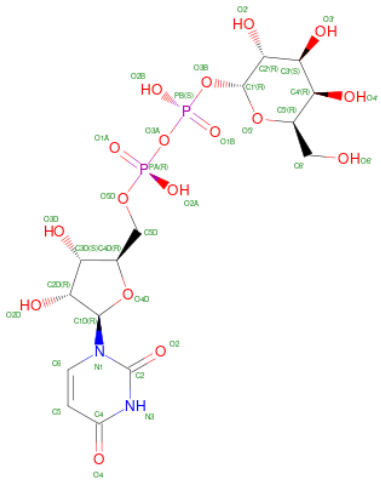
FAD



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

- Molecule 3 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).

GDU



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	36	15	2	17	2	0	0
3	B	1	36	15	2	17	2	0	0
3	C	1	36	15	2	17	2	0	0
3	D	1	36	15	2	17	2	0	0

- Molecule 4 is water.

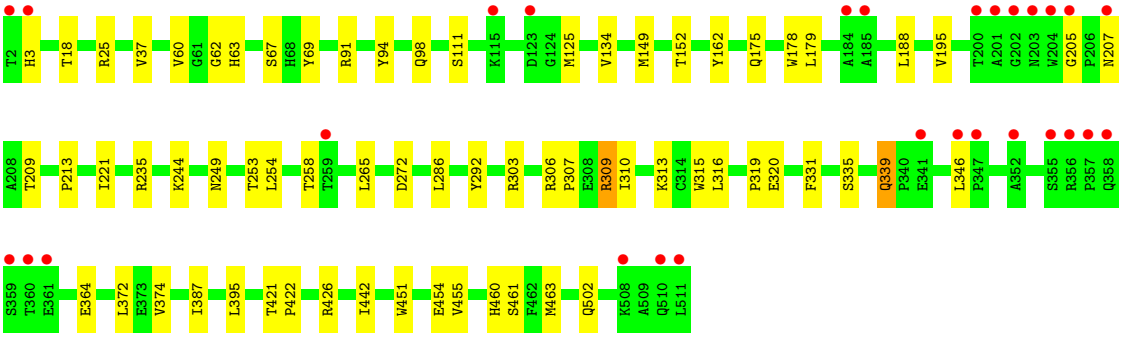
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	20	20	20	0	0
4	B	25	25	25	0	0
4	C	15	15	15	0	0
4	D	9	9	9	0	0

3 Residue-property plots (i)

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

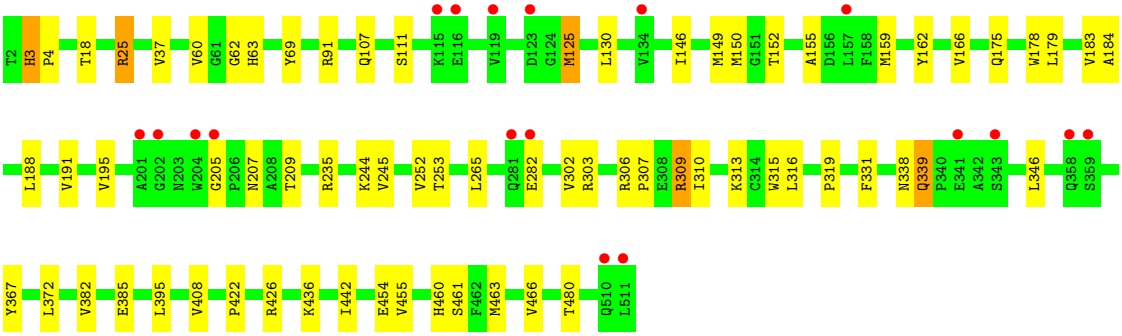
• Molecule 1: UDP-galactopyranose mutase

Chain A:



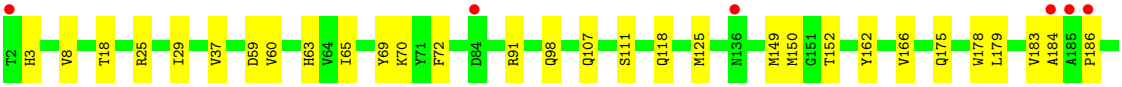
• Molecule 1: UDP-galactopyranose mutase

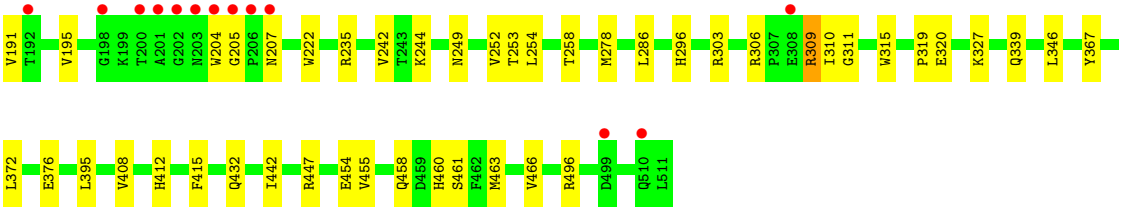
Chain B:



• Molecule 1: UDP-galactopyranose mutase

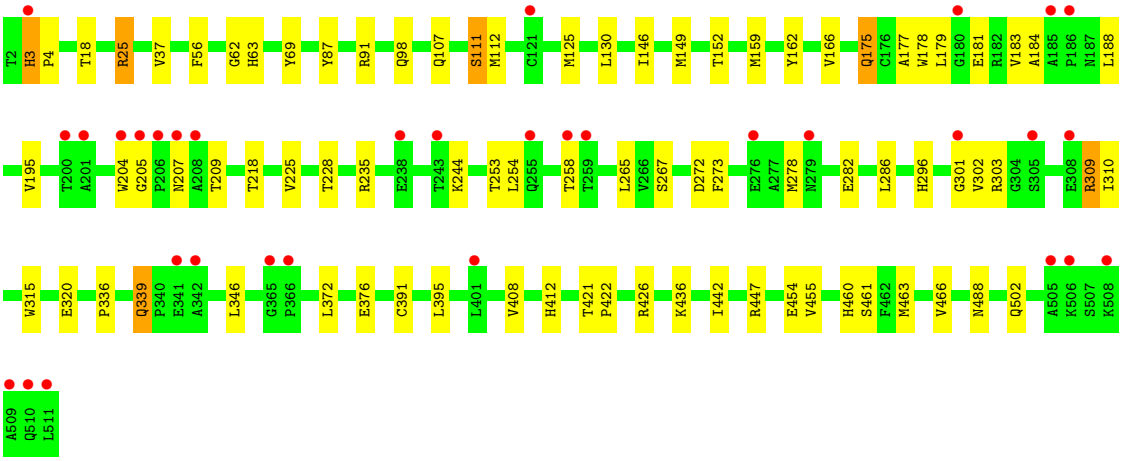
Chain C:





- Molecule 1: UDP-galactopyranose mutase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	129.54Å 135.48Å 176.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.15 48.69 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 ((Not available)-3.15) 99.8 (48.69-3.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.212 , 0.248 0.202 , 0.241	Depositor DCC
R_{free} test set	2709 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.910	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16433	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3192e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GDU, 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	0.25	0/4101	0.42	0/5573
1	B	0.24	0/4101	0.42	0/5573
1	C	0.25	0/4101	0.43	0/5573
1	D	0.24	0/4101	0.43	0/5573
All	All	0.25	0/16404	0.42	0/22292

There are no bond length outliers.

There are no bond angle outliers.

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	4002	0	3925	34	0
1	B	4002	0	3925	40	0
1	C	4002	0	3925	51	0
1	D	4002	0	3925	45	0
2	A	53	0	30	0	0
2	B	53	0	30	0	0
2	C	53	0	30	0	0
2	D	53	0	30	1	0
3	A	36	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	22	2	0
3	C	36	0	22	5	0
3	D	36	0	22	2	0
4	A	20	0	0	1	0
4	B	25	0	0	1	0
4	C	15	0	0	1	0
4	D	9	0	0	1	0
All	All	16433	0	15908	169	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 5.

All (169) 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:244:LYS:HB3	1:A:253:THR:HB	1.64	0.80
1:C:278:MET:HE1	1:C:442:ILE:HD13	1.62	0.79
1:D:244:LYS:HB3	1:D:253:THR:HB	1.68	0.76
1:D:91:ARG:HH12	1:D:205:GLY:HA3	1.49	0.75
1:B:244:LYS:HB3	1:B:253:THR:HB	1.71	0.73
1:D:303:ARG:NH2	1:D:346:LEU:O	2.23	0.71
1:D:91:ARG:HD3	1:D:207:ASN:HB2	1.72	0.69
1:C:91:ARG:HD3	1:C:207:ASN:HB2	1.76	0.68
1:A:303:ARG:NH2	1:A:346:LEU:O	2.25	0.68
1:D:296:HIS:HD2	1:D:412:HIS:HE1	1.42	0.66
1:C:69:TYR:CG	1:C:463:MET:HG3	2.31	0.65
1:C:303:ARG:NH2	1:C:346:LEU:O	2.21	0.65
1:A:69:TYR:CG	1:A:463:MET:HG3	2.32	0.64
1:B:91:ARG:HH12	1:B:205:GLY:HA3	1.63	0.63
1:D:107:GLN:HE21	1:D:184:ALA:HB3	1.63	0.63
1:B:303:ARG:NH2	1:B:346:LEU:O	2.29	0.61
1:A:309:ARG:HG2	1:A:310:ILE:HD12	1.83	0.61
1:D:69:TYR:CG	1:D:463:MET:HG3	2.35	0.61
1:B:69:TYR:CG	1:B:463:MET:HG3	2.36	0.60
1:C:111:SER:HA	1:C:118:GLN:HE21	1.68	0.59
1:B:107:GLN:HE21	1:B:184:ALA:HB3	1.68	0.59
1:C:296:HIS:HD2	1:C:412:HIS:HE1	1.51	0.59
1:A:455:VAL:HG22	1:A:460:HIS:HB3	1.84	0.58
1:D:309:ARG:HG2	1:D:310:ILE:HD12	1.84	0.58
1:B:338:ASN:HB2	1:B:339:GLN:HE21	1.69	0.58
1:C:91:ARG:HH12	1:C:205:GLY:HA3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:VAL:O	1:D:228:THR:OG1	2.22	0.57
1:D:502:GLN:NE2	4:D:703:HOH:O	2.37	0.57
1:D:178:TRP:HB2	1:D:454:GLU:HG3	1.86	0.57
1:D:372:LEU:HD21	1:D:395:LEU:HD21	1.87	0.57
1:C:183:VAL:HG22	3:C:602:GDU:H1D	1.85	0.57
1:A:91:ARG:HD3	1:A:207:ASN:HB2	1.87	0.56
1:B:265:LEU:HB3	1:B:442:ILE:HG12	1.86	0.56
1:A:111:SER:HB3	1:A:195:VAL:HA	1.88	0.56
1:B:91:ARG:HD3	1:B:207:ASN:HB2	1.87	0.56
1:D:183:VAL:HG22	3:D:602:GDU:H1D	1.86	0.56
1:A:374:VAL:HG11	1:A:387:ILE:HD11	1.89	0.55
1:A:265:LEU:HB3	1:A:442:ILE:HG12	1.89	0.55
1:B:309:ARG:HG2	1:B:310:ILE:HD12	1.89	0.55
1:B:183:VAL:HG22	3:B:602:GDU:H1D	1.88	0.54
1:D:63:HIS:HB2	1:D:218:THR:HG21	1.89	0.54
1:A:335:SER:O	1:A:339:GLN:NE2	2.41	0.53
1:B:245:VAL:HG22	1:B:252:VAL:HG22	1.92	0.52
1:B:125:MET:HB3	1:B:188:LEU:HD13	1.92	0.52
1:C:178:TRP:HB2	1:C:454:GLU:HG3	1.91	0.52
1:B:18:THR:OG1	1:B:461:SER:HB3	2.09	0.52
1:C:372:LEU:HD21	1:C:395:LEU:HD21	1.91	0.52
1:A:91:ARG:HH12	1:A:205:GLY:HA3	1.74	0.52
1:D:278:MET:HE1	1:D:442:ILE:HD13	1.92	0.52
1:C:254:LEU:HD12	1:C:258:THR:HB	1.92	0.51
1:D:98:GLN:N	1:D:320:GLU:OE1	2.38	0.51
1:B:282:GLU:OE2	1:B:436:LYS:NZ	2.36	0.51
1:C:18:THR:OG1	1:C:461:SER:HB3	2.11	0.51
1:C:296:HIS:HE1	1:C:376:GLU:OE2	1.94	0.50
1:D:460:HIS:NE2	1:D:488:ASN:OD1	2.44	0.50
1:A:18:THR:OG1	1:A:461:SER:HB3	2.12	0.50
1:A:272:ASP:OD1	1:A:272:ASP:N	2.44	0.49
1:B:60:VAL:O	1:B:63:HIS:NE2	2.44	0.49
1:C:309:ARG:HG2	1:C:310:ILE:HD12	1.94	0.49
1:B:91:ARG:HG3	1:B:315:TRP:CH2	2.48	0.49
1:A:502:GLN:NE2	4:A:704:HOH:O	2.44	0.49
1:B:455:VAL:HG22	1:B:460:HIS:HB3	1.94	0.49
1:D:25:ARG:HD2	1:D:466:VAL:HG13	1.95	0.49
1:B:175:GLN:NE2	4:B:710:HOH:O	2.45	0.49
1:C:162:TYR:O	1:C:166:VAL:HG12	2.13	0.49
1:D:18:THR:OG1	1:D:461:SER:HB3	2.14	0.48
1:A:37:VAL:HG12	1:A:235:ARG:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:VAL:HG21	1:B:480:THR:HG23	1.95	0.48
1:B:178:TRP:HB2	1:B:454:GLU:HG3	1.96	0.48
1:C:455:VAL:HG22	1:C:460:HIS:HB3	1.94	0.48
1:C:447:ARG:NH1	4:C:701:HOH:O	2.43	0.48
1:A:426:ARG:NH1	1:A:454:GLU:OE2	2.42	0.48
1:B:162:TYR:HB2	1:B:319:PRO:HB3	1.96	0.48
1:A:91:ARG:HG3	1:A:315:TRP:CH2	2.49	0.48
1:B:315:TRP:CE2	3:B:602:GDU:H6'2	2.49	0.47
1:B:155:ALA:HA	1:B:159:MET:HB2	1.96	0.47
1:A:125:MET:HB3	1:A:188:LEU:HD13	1.95	0.47
1:C:296:HIS:CD2	1:C:412:HIS:HE1	2.32	0.47
1:D:91:ARG:NH2	1:D:204:TRP:O	2.39	0.47
1:D:315:TRP:CE2	3:D:602:GDU:H6'2	2.50	0.47
1:C:162:TYR:HB2	1:C:319:PRO:HB3	1.97	0.47
1:D:125:MET:HB3	1:D:188:LEU:HD13	1.96	0.47
1:C:98:GLN:N	1:C:320:GLU:OE1	2.37	0.47
1:D:162:TYR:O	1:D:166:VAL:HG12	2.15	0.47
1:B:37:VAL:HG12	1:B:235:ARG:HB3	1.97	0.46
1:C:60:VAL:O	1:C:63:HIS:NE2	2.48	0.46
1:C:286:LEU:HD21	1:C:432:GLN:HB3	1.98	0.46
1:D:296:HIS:HE1	1:D:376:GLU:OE2	1.98	0.46
1:C:327:LYS:NZ	3:C:602:GDU:C1'	2.78	0.46
1:D:282:GLU:OE2	1:D:436:LYS:NZ	2.42	0.46
1:D:455:VAL:HG22	1:D:460:HIS:HB3	1.98	0.46
1:D:422:PRO:HA	1:D:426:ARG:HD3	1.98	0.46
1:A:98:GLN:N	1:A:320:GLU:OE1	2.32	0.46
1:C:60:VAL:HB	1:C:63:HIS:HE2	1.81	0.46
1:C:244:LYS:HB3	1:C:253:THR:HB	1.98	0.46
1:B:175:GLN:HG3	1:B:178:TRP:HD1	1.81	0.46
1:D:254:LEU:HD12	1:D:258:THR:HB	1.96	0.45
1:D:265:LEU:HB3	1:D:442:ILE:HG12	1.98	0.45
1:C:327:LYS:NZ	3:C:602:GDU:O5'	2.49	0.45
1:C:367:TYR:HE1	1:C:408:VAL:HG21	1.81	0.45
1:C:296:HIS:HD2	1:C:412:HIS:CE1	2.34	0.45
1:D:146:ILE:HD13	1:D:159:MET:HB3	1.98	0.45
1:D:175:GLN:HG2	1:D:177:ALA:H	1.82	0.45
1:D:447:ARG:HD2	2:D:601:FAD:O3'	2.17	0.45
1:C:25:ARG:O	1:C:29:ILE:HG13	2.17	0.44
1:D:272:ASP:OD1	1:D:273:PHE:N	2.50	0.44
1:D:426:ARG:NH2	1:D:454:GLU:OE1	2.36	0.44
1:C:175:GLN:HG3	1:C:178:TRP:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:VAL:HG13	1:C:252:VAL:HG13	1.99	0.44
1:C:25:ARG:HD2	1:C:466:VAL:HG13	1.99	0.44
1:B:146:ILE:HD13	1:B:159:MET:HB3	2.00	0.44
1:A:315:TRP:CE2	3:A:602:GDU:H6'2	2.52	0.44
1:B:3:HIS:HA	1:B:4:PRO:HD3	1.84	0.44
1:A:178:TRP:HB2	1:A:454:GLU:HG3	1.99	0.44
1:C:91:ARG:HB2	1:C:207:ASN:O	2.17	0.44
1:C:125:MET:HG2	1:C:150:MET:O	2.18	0.44
1:A:292:TYR:HB3	1:A:451:TRP:CZ2	2.53	0.44
1:A:421:THR:HA	1:A:422:PRO:HD3	1.86	0.44
1:C:327:LYS:NZ	3:C:602:GDU:O3B	2.50	0.44
1:C:306:ARG:HD2	1:C:311:GLY:O	2.17	0.43
1:A:254:LEU:HD12	1:A:258:THR:HB	2.01	0.43
1:A:372:LEU:HD21	1:A:395:LEU:HD21	2.00	0.43
1:C:107:GLN:HE21	1:C:184:ALA:HB3	1.83	0.43
1:C:37:VAL:HG12	1:C:235:ARG:HB3	1.99	0.43
1:B:426:ARG:NH1	1:B:454:GLU:OE2	2.45	0.43
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.54	0.43
1:D:37:VAL:HG12	1:D:235:ARG:HB3	2.00	0.43
1:C:184:ALA:HB2	1:C:204:TRP:CE3	2.54	0.43
1:C:70:LYS:HG2	1:C:496:ARG:CZ	2.49	0.43
1:C:367:TYR:CE1	1:C:408:VAL:HG21	2.54	0.43
1:A:60:VAL:O	1:A:63:HIS:NE2	2.51	0.42
1:A:313:LYS:HD3	1:A:316:LEU:HD21	2.01	0.42
1:B:25:ARG:HD2	1:B:466:VAL:HG13	2.01	0.42
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.54	0.42
1:B:130:LEU:HD23	1:D:130:LEU:HD23	2.01	0.42
1:A:91:ARG:HB2	1:A:207:ASN:O	2.19	0.42
1:A:306:ARG:HA	1:A:307:PRO:HD3	1.91	0.42
1:B:191:VAL:O	1:B:195:VAL:HG23	2.20	0.42
1:B:313:LYS:HD3	1:B:316:LEU:HD21	2.01	0.42
1:B:422:PRO:HA	1:B:426:ARG:HD3	2.01	0.42
1:D:184:ALA:HB2	1:D:204:TRP:CE3	2.55	0.42
1:C:65:ILE:HD11	1:C:458:GLN:HE22	1.85	0.42
1:D:421:THR:HA	1:D:422:PRO:HD3	1.83	0.42
1:D:111:SER:HB3	1:D:195:VAL:HA	2.01	0.41
1:C:72:PHE:HE1	1:C:222:TRP:HH2	1.68	0.41
1:C:91:ARG:NH2	1:C:204:TRP:O	2.45	0.41
1:D:463:MET:HA	1:D:466:VAL:HB	2.03	0.41
1:A:94:TYR:HB2	1:A:316:LEU:HD22	2.03	0.41
1:C:60:VAL:HG13	1:C:415:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HG3	1:C:315:TRP:CH2	2.56	0.41
1:C:150:MET:HG2	1:C:186:PRO:HG3	2.03	0.41
1:A:213:PRO:HD3	1:A:221:ILE:HD11	2.03	0.41
1:C:69:TYR:CD2	1:C:463:MET:HG3	2.56	0.41
1:C:183:VAL:HG13	3:C:602:GDU:O2	2.21	0.41
1:B:162:TYR:O	1:B:166:VAL:HG12	2.21	0.41
1:D:301:GLY:O	1:D:408:VAL:N	2.46	0.41
1:B:367:TYR:HE1	1:B:408:VAL:HG21	1.85	0.41
1:A:162:TYR:HB2	1:A:319:PRO:HB3	2.03	0.41
1:A:175:GLN:HG3	1:A:178:TRP:HD1	1.86	0.41
1:B:125:MET:HG2	1:B:150:MET:O	2.21	0.41
1:D:87:TYR:CE2	1:D:336:PRO:HD2	2.55	0.41
1:A:69:TYR:CD1	1:A:463:MET:HG3	2.57	0.40
1:B:91:ARG:HB2	1:B:207:ASN:O	2.20	0.40
1:D:372:LEU:HD12	1:D:391:CYS:HB3	2.03	0.40
1:B:372:LEU:HD21	1:B:395:LEU:HD21	2.03	0.40
1:D:3:HIS:HA	1:D:4:PRO:HD3	1.91	0.40
1:B:306:ARG:HA	1:B:307:PRO:HD3	1.93	0.40
1:C:191:VAL:O	1:C:195:VAL:HG23	2.21	0.40
1:D:56:PHE:CE1	1:D:339:GLN:HB3	2.55	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	508/510 (100%)	485 (96%)	22 (4%)	1 (0%)	47	78
1	B	508/510 (100%)	488 (96%)	19 (4%)	1 (0%)	47	78
1	C	508/510 (100%)	491 (97%)	16 (3%)	1 (0%)	47	78
1	D	508/510 (100%)	488 (96%)	19 (4%)	1 (0%)	47	78
All	All	2032/2040 (100%)	1952 (96%)	76 (4%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLY
1	B	62	GLY
1	C	59	ASP
1	D	62	GLY

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	432/432 (100%)	418 (97%)	14 (3%)	39	70
1	B	432/432 (100%)	418 (97%)	14 (3%)	39	70
1	C	432/432 (100%)	424 (98%)	8 (2%)	57	80
1	D	432/432 (100%)	417 (96%)	15 (4%)	36	67
All	All	1728/1728 (100%)	1677 (97%)	51 (3%)	41	71

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	25	ARG
1	A	67	SER
1	A	134	VAL
1	A	149	MET
1	A	152	THR
1	A	179	LEU
1	A	209	THR
1	A	249	ASN
1	A	286	LEU
1	A	309	ARG
1	A	331	PHE
1	A	339	GLN
1	A	364	GLU
1	B	3	HIS
1	B	25	ARG

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Mol	Chain	Res	Type
1	B	111	SER
1	B	125	MET
1	B	149	MET
1	B	152	THR
1	B	179	LEU
1	B	209	THR
1	B	302	VAL
1	B	309	ARG
1	B	331	PHE
1	B	339	GLN
1	B	382	VAL
1	B	385	GLU
1	C	3	HIS
1	C	8	VAL
1	C	149	MET
1	C	152	THR
1	C	179	LEU
1	C	249	ASN
1	C	309	ARG
1	C	339	GLN
1	D	3	HIS
1	D	25	ARG
1	D	111	SER
1	D	112	MET
1	D	149	MET
1	D	152	THR
1	D	175	GLN
1	D	179	LEU
1	D	181	GLU
1	D	209	THR
1	D	267	SER
1	D	286	LEU
1	D	302	VAL
1	D	309	ARG
1	D	339	GLN

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

Mol	Chain	Res	Type
1	B	339	GLN
1	C	296	HIS
1	C	350	GLN

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Mol	Chain	Res	Type
1	C	412	HIS
1	C	458	GLN
1	D	175	GLN
1	D	296	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	GDU	C	602	-	35,38,38	1.88	11 (31%)	53,58,58	2.02	12 (22%)
3	GDU	D	602	-	35,38,38	1.87	11 (31%)	53,58,58	1.91	12 (22%)
2	FAD	C	601	-	53,58,58	2.49	16 (30%)	68,89,89	1.70	16 (23%)
3	GDU	B	602	-	35,38,38	1.88	11 (31%)	53,58,58	1.92	12 (22%)
2	FAD	D	601	-	53,58,58	2.48	16 (30%)	68,89,89	1.72	17 (25%)
2	FAD	B	601	-	53,58,58	2.48	16 (30%)	68,89,89	1.69	17 (25%)
3	GDU	A	602	-	35,38,38	1.87	11 (31%)	53,58,58	1.95	14 (26%)
2	FAD	A	601	-	53,58,58	2.47	16 (30%)	68,89,89	1.72	15 (22%)

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
3	GDU	C	602	-	-	13/23/59/59	0/3/3/3
3	GDU	D	602	-	-	11/23/59/59	0/3/3/3
2	FAD	C	601	-	-	11/30/50/50	0/6/6/6
3	GDU	B	602	-	-	12/23/59/59	0/3/3/3
2	FAD	D	601	-	-	13/30/50/50	0/6/6/6
2	FAD	B	601	-	-	15/30/50/50	0/6/6/6
3	GDU	A	602	-	-	15/23/59/59	0/3/3/3
2	FAD	A	601	-	-	6/30/50/50	0/6/6/6

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	O4-C4	10.44	1.43	1.23
2	D	601	FAD	O4-C4	10.35	1.43	1.23
2	B	601	FAD	O4-C4	10.27	1.43	1.23
2	A	601	FAD	O4-C4	10.27	1.43	1.23
2	C	601	FAD	O2-C2	7.57	1.38	1.24
2	A	601	FAD	O2-C2	7.53	1.38	1.24
2	D	601	FAD	O2-C2	7.46	1.38	1.24
2	B	601	FAD	O2-C2	7.23	1.37	1.24
2	D	601	FAD	C2B-C3B	-4.90	1.39	1.53
2	C	601	FAD	C2B-C3B	-4.80	1.40	1.53
2	B	601	FAD	C2B-C3B	-4.79	1.40	1.53
3	B	602	GDU	O4-C4	4.76	1.33	1.24
3	D	602	GDU	O4-C4	4.73	1.33	1.24
3	A	602	GDU	O4-C4	4.71	1.33	1.24
3	C	602	GDU	O4-C4	4.71	1.33	1.24
2	A	601	FAD	C2B-C3B	-4.64	1.40	1.53
2	A	601	FAD	C1'-C2'	-4.04	1.47	1.52
2	B	601	FAD	C5'-C4'	-3.96	1.46	1.51
2	C	601	FAD	C1'-C2'	-3.96	1.47	1.52
2	B	601	FAD	C1'-C2'	-3.93	1.47	1.52
2	D	601	FAD	C1'-C2'	-3.78	1.47	1.52
3	D	602	GDU	PB-O3B	-3.78	1.50	1.60
3	A	602	GDU	PB-O3B	-3.77	1.50	1.60
2	D	601	FAD	C5'-C4'	-3.75	1.46	1.51
3	C	602	GDU	PB-O3B	-3.70	1.50	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	GDU	PB-O3B	-3.66	1.50	1.60
2	C	601	FAD	C5'-C4'	-3.59	1.46	1.51
2	A	601	FAD	C5'-C4'	-3.45	1.46	1.51
2	D	601	FAD	O2'-C2'	-3.42	1.36	1.43
2	C	601	FAD	O2'-C2'	-3.35	1.36	1.43
2	B	601	FAD	O2'-C2'	-3.33	1.36	1.43
3	A	602	GDU	C3D-C2D	-3.29	1.44	1.53
2	B	601	FAD	C9A-N10	-3.26	1.35	1.41
3	B	602	GDU	C3D-C2D	-3.19	1.44	1.53
3	C	602	GDU	C3D-C2D	-3.14	1.44	1.53
2	C	601	FAD	C2B-C1B	-3.12	1.49	1.53
2	A	601	FAD	C9A-N10	-3.12	1.35	1.41
2	A	601	FAD	O2'-C2'	-3.11	1.36	1.43
3	B	602	GDU	C4'-C3'	-3.09	1.44	1.52
2	D	601	FAD	C2B-C1B	-3.05	1.49	1.53
2	B	601	FAD	C2B-C1B	-3.05	1.49	1.53
2	C	601	FAD	C9A-N10	-3.04	1.35	1.41
3	D	602	GDU	C3D-C2D	-3.01	1.45	1.53
2	A	601	FAD	C2B-C1B	-3.00	1.49	1.53
3	D	602	GDU	C4'-C3'	-2.87	1.45	1.52
3	C	602	GDU	C3D-C4D	-2.81	1.45	1.53
3	A	602	GDU	C3D-C4D	-2.80	1.45	1.53
3	B	602	GDU	C3D-C4D	-2.79	1.45	1.53
2	D	601	FAD	C7M-C7	2.79	1.56	1.51
3	C	602	GDU	C4'-C3'	-2.76	1.45	1.52
2	B	601	FAD	C4-N3	-2.74	1.33	1.38
3	D	602	GDU	C4-N3	-2.73	1.33	1.38
3	A	602	GDU	C4'-C3'	-2.73	1.45	1.52
2	A	601	FAD	C7M-C7	2.73	1.56	1.51
3	C	602	GDU	C4-N3	-2.72	1.33	1.38
2	A	601	FAD	PA-O1A	-2.69	1.41	1.50
3	D	602	GDU	C3D-C4D	-2.67	1.46	1.53
3	A	602	GDU	C4-N3	-2.66	1.33	1.38
2	D	601	FAD	PA-O1A	-2.66	1.41	1.50
2	B	601	FAD	PA-O1A	-2.65	1.41	1.50
3	B	602	GDU	C4-N3	-2.64	1.33	1.38
2	B	601	FAD	C7M-C7	2.64	1.56	1.51
3	D	602	GDU	C2-N1	-2.63	1.34	1.38
2	D	601	FAD	C9A-N10	-2.62	1.36	1.41
2	D	601	FAD	C4-N3	-2.60	1.34	1.38
2	C	601	FAD	PA-O1A	-2.57	1.41	1.50
3	C	602	GDU	C2-N1	-2.57	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C4-N3	-2.56	1.34	1.38
3	A	602	GDU	C2-N1	-2.54	1.34	1.38
2	A	601	FAD	C4-N3	-2.54	1.34	1.38
2	C	601	FAD	C7M-C7	2.52	1.56	1.51
3	B	602	GDU	C2-N1	-2.47	1.34	1.38
3	C	602	GDU	O5'-C5'	2.36	1.50	1.44
2	D	601	FAD	O4B-C4B	-2.31	1.39	1.45
3	C	602	GDU	C3'-C2'	-2.30	1.46	1.52
2	A	601	FAD	O4B-C1B	-2.29	1.37	1.41
3	B	602	GDU	O5'-C5'	2.26	1.49	1.44
3	C	602	GDU	C6-C5	2.26	1.40	1.35
2	B	601	FAD	O4B-C4B	-2.25	1.40	1.45
2	A	601	FAD	O4B-C4B	-2.24	1.40	1.45
3	A	602	GDU	O5'-C5'	2.24	1.49	1.44
3	D	602	GDU	O5'-C5'	2.24	1.49	1.44
3	B	602	GDU	C6-C5	2.23	1.40	1.35
3	D	602	GDU	C6-C5	2.23	1.40	1.35
3	D	602	GDU	C3'-C2'	-2.22	1.46	1.52
2	C	601	FAD	O4B-C4B	-2.21	1.40	1.45
3	A	602	GDU	C6-C5	2.20	1.40	1.35
3	A	602	GDU	C3'-C2'	-2.19	1.46	1.52
3	B	602	GDU	C3'-C2'	-2.18	1.46	1.52
2	A	601	FAD	C6A-N6A	2.17	1.41	1.34
2	B	601	FAD	C6A-N6A	2.16	1.41	1.34
2	C	601	FAD	C6A-N6A	2.16	1.41	1.34
2	D	601	FAD	C6A-N6A	2.14	1.41	1.34
2	B	601	FAD	C3B-C4B	-2.14	1.47	1.53
3	A	602	GDU	C5-C4	-2.14	1.38	1.43
2	A	601	FAD	C4X-N5	2.12	1.34	1.30
2	C	601	FAD	O4B-C1B	-2.11	1.38	1.41
2	D	601	FAD	C3B-C4B	-2.10	1.47	1.53
2	B	601	FAD	O4B-C1B	-2.10	1.38	1.41
2	C	601	FAD	C3B-C4B	-2.09	1.47	1.53
3	D	602	GDU	C5-C4	-2.08	1.39	1.43
3	B	602	GDU	C5-C4	-2.07	1.39	1.43
2	A	601	FAD	C3B-C4B	-2.07	1.47	1.53
3	C	602	GDU	C5-C4	-2.05	1.39	1.43
2	D	601	FAD	O4B-C1B	-2.05	1.38	1.41
2	D	601	FAD	C2'-C3'	-2.04	1.49	1.53
2	B	601	FAD	C2'-C3'	-2.03	1.49	1.53
2	C	601	FAD	C4X-N5	2.00	1.34	1.30

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	GDU	N3-C2-N1	6.36	123.33	114.89
3	B	602	GDU	N3-C2-N1	6.29	123.24	114.89
3	D	602	GDU	N3-C2-N1	6.01	122.87	114.89
3	A	602	GDU	N3-C2-N1	5.94	122.77	114.89
3	C	602	GDU	C4-N3-C2	-5.39	119.47	126.58
3	B	602	GDU	C4-N3-C2	-5.34	119.54	126.58
3	A	602	GDU	C4-N3-C2	-5.12	119.82	126.58
3	D	602	GDU	C4-N3-C2	-5.10	119.86	126.58
2	C	601	FAD	N3A-C2A-N1A	-5.04	120.81	128.68
2	D	601	FAD	O2'-C2'-C1'	4.85	121.52	109.80
2	A	601	FAD	N3A-C2A-N1A	-4.68	121.36	128.68
2	C	601	FAD	C1B-N9A-C4A	-4.65	118.48	126.64
2	B	601	FAD	N3A-C2A-N1A	-4.63	121.45	128.68
2	D	601	FAD	N3A-C2A-N1A	-4.61	121.48	128.68
2	A	601	FAD	C1B-N9A-C4A	-4.42	118.88	126.64
2	A	601	FAD	O5'-C5'-C4'	4.38	121.06	109.36
2	B	601	FAD	O2'-C2'-C1'	4.30	120.19	109.80
3	C	602	GDU	O5'-C5'-C4'	4.23	117.37	109.69
3	C	602	GDU	C3'-C4'-C5'	4.22	117.76	110.24
2	D	601	FAD	C1B-N9A-C4A	-4.15	119.35	126.64
2	C	601	FAD	O2'-C2'-C1'	4.10	119.71	109.80
2	B	601	FAD	C1B-N9A-C4A	-4.09	119.45	126.64
3	A	602	GDU	C3'-C4'-C5'	3.99	117.36	110.24
3	D	602	GDU	PB-O3A-PA	-3.95	119.26	132.83
3	D	602	GDU	O5'-C5'-C4'	3.93	116.84	109.69
3	D	602	GDU	C3'-C4'-C5'	3.88	117.16	110.24
3	C	602	GDU	PB-O3A-PA	-3.80	119.78	132.83
3	B	602	GDU	PB-O3A-PA	-3.79	119.82	132.83
3	A	602	GDU	PB-O3A-PA	-3.78	119.86	132.83
2	D	601	FAD	O2'-C2'-C3'	3.75	118.22	109.10
2	C	601	FAD	O2'-C2'-C3'	3.74	118.19	109.10
3	A	602	GDU	O5'-C5'-C4'	3.67	116.36	109.69
2	A	601	FAD	O2'-C2'-C1'	3.65	118.63	109.80
2	B	601	FAD	O2'-C2'-C3'	3.49	117.58	109.10
2	D	601	FAD	P-O3P-PA	-3.47	120.93	132.83
2	A	601	FAD	O2'-C2'-C3'	3.43	117.45	109.10
3	B	602	GDU	O2-C2-N1	-3.37	118.30	122.79
2	B	601	FAD	C4-N3-C2	-3.36	119.43	125.64
2	A	601	FAD	P-O3P-PA	-3.35	121.33	132.83
3	C	602	GDU	O2-C2-N1	-3.29	118.42	122.79
3	B	602	GDU	O5'-C5'-C4'	3.21	115.52	109.69
3	D	602	GDU	O2-C2-N1	-3.19	118.55	122.79
2	D	601	FAD	O5'-C5'-C4'	3.17	117.82	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	GDU	O2-C2-N1	-3.15	118.60	122.79
3	D	602	GDU	C5-C4-N3	3.14	119.54	114.84
3	A	602	GDU	C5-C4-N3	3.14	119.54	114.84
2	D	601	FAD	C4X-C10-N10	3.12	121.05	116.48
2	C	601	FAD	O5'-C5'-C4'	3.11	117.65	109.36
2	A	601	FAD	C4-C4X-N5	3.09	122.64	118.23
3	C	602	GDU	C5-C4-N3	3.09	119.47	114.84
2	C	601	FAD	C4-N3-C2	-3.06	119.99	125.64
2	D	601	FAD	C4-C4X-N5	3.04	122.56	118.23
2	A	601	FAD	C4-N3-C2	-3.04	120.03	125.64
3	B	602	GDU	C5-C4-N3	3.01	119.34	114.84
3	B	602	GDU	C3'-C4'-C5'	3.00	115.60	110.24
3	C	602	GDU	O3B-C1'-C2'	2.98	113.84	108.38
2	A	601	FAD	C4X-C4-N3	2.98	120.76	113.19
2	B	601	FAD	C4X-C4-N3	2.89	120.54	113.19
2	C	601	FAD	C4-C4X-N5	2.87	122.32	118.23
2	C	601	FAD	O5B-C5B-C4B	2.82	118.70	108.99
2	C	601	FAD	C4X-C4-N3	2.80	120.30	113.19
2	B	601	FAD	O5B-C5B-C4B	2.78	118.55	108.99
2	B	601	FAD	O5'-C5'-C4'	2.77	116.76	109.36
3	B	602	GDU	O4-C4-C5	-2.75	120.33	125.16
2	D	601	FAD	C4-N3-C2	-2.74	120.57	125.64
3	A	602	GDU	O4-C4-C5	-2.74	120.35	125.16
2	D	601	FAD	C4X-C4-N3	2.72	120.11	113.19
2	B	601	FAD	C4-C4X-N5	2.71	122.08	118.23
3	A	602	GDU	C3D-C2D-C1D	2.70	106.55	101.43
2	B	601	FAD	C4X-C10-N10	2.67	120.38	116.48
3	D	602	GDU	C3D-C2D-C1D	2.66	106.48	101.43
3	C	602	GDU	O4-C4-C5	-2.63	120.53	125.16
3	B	602	GDU	O3B-C1'-C2'	2.63	113.20	108.38
3	A	602	GDU	O3A-PB-O3B	2.63	107.78	102.48
2	B	601	FAD	C4A-C5A-N7A	-2.62	106.66	109.40
3	D	602	GDU	O4-C4-C5	-2.60	120.59	125.16
3	B	602	GDU	O4D-C1D-N1	2.59	114.29	108.36
2	A	601	FAD	O4-C4-C4X	-2.59	119.72	126.60
2	D	601	FAD	O5B-C5B-C4B	2.58	117.89	108.99
2	A	601	FAD	C4'-C3'-C2'	2.55	118.68	113.36
2	A	601	FAD	O5B-C5B-C4B	2.50	117.58	108.99
3	B	602	GDU	C3D-C2D-C1D	2.49	106.17	101.43
2	C	601	FAD	C4X-C10-N10	2.49	120.12	116.48
2	D	601	FAD	O4-C4-C4X	-2.42	120.19	126.60
3	C	602	GDU	C3D-C2D-C1D	2.41	106.01	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	O4-C4-C4X	-2.41	120.20	126.60
2	C	601	FAD	O4-C4-C4X	-2.39	120.27	126.60
2	D	601	FAD	C1'-C2'-C3'	2.38	116.45	109.79
2	C	601	FAD	P-O3P-PA	-2.38	124.67	132.83
2	D	601	FAD	C4A-C5A-N7A	-2.36	106.94	109.40
2	B	601	FAD	O4'-C4'-C3'	2.36	114.83	109.10
2	C	601	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
2	C	601	FAD	C10-C4X-N5	-2.31	119.96	124.86
3	C	602	GDU	O4D-C1D-N1	2.30	113.63	108.36
2	D	601	FAD	C1'-N10-C9A	2.30	124.35	120.51
2	C	601	FAD	C1'-C2'-C3'	2.28	116.17	109.79
3	A	602	GDU	O3B-C1'-C2'	2.25	112.50	108.38
2	A	601	FAD	C4A-C5A-N7A	-2.24	107.07	109.40
3	B	602	GDU	O3A-PB-O3B	2.24	106.99	102.48
2	B	601	FAD	P-O3P-PA	-2.21	125.24	132.83
2	A	601	FAD	C4X-C10-N10	2.20	119.69	116.48
3	A	602	GDU	C4'-C3'-C2'	2.19	114.65	110.82
3	D	602	GDU	O3A-PB-O3B	2.19	106.90	102.48
3	D	602	GDU	O3B-C1'-C2'	2.16	112.33	108.38
2	B	601	FAD	C10-C4X-N5	-2.16	120.28	124.86
2	C	601	FAD	C4X-C10-N1	-2.15	119.75	124.73
2	A	601	FAD	C10-C4X-N5	-2.14	120.32	124.86
2	B	601	FAD	O4B-C1B-C2B	-2.14	103.81	106.93
2	B	601	FAD	C4X-C10-N1	-2.13	119.80	124.73
3	C	602	GDU	O3A-PB-O3B	2.12	106.76	102.48
2	D	601	FAD	C10-C4X-N5	-2.08	120.45	124.86
2	D	601	FAD	C3B-C2B-C1B	2.06	104.08	100.98
3	A	602	GDU	O4D-C1D-N1	2.04	113.03	108.36
3	D	602	GDU	O4D-C1D-N1	2.04	113.03	108.36
3	A	602	GDU	O5D-C5D-C4D	2.01	115.91	108.99

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	P-O3P-PA-O5B
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	C	601	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	601	FAD	C5B-O5B-PA-O2A
2	C	601	FAD	C1'-C2'-C3'-O3'
2	C	601	FAD	C1'-C2'-C3'-C4'
2	C	601	FAD	C3'-C4'-C5'-O5'
2	C	601	FAD	O4'-C4'-C5'-O5'
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C2'-C1'-N10-C10
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	N10-C1'-C2'-C3'
2	D	601	FAD	C1'-C2'-C3'-O3'
2	D	601	FAD	C1'-C2'-C3'-C4'
3	A	602	GDU	C3D-C4D-C5D-O5D
3	A	602	GDU	O4D-C4D-C5D-O5D
3	A	602	GDU	C5D-O5D-PA-O3A
3	A	602	GDU	PA-O3A-PB-O3B
3	A	602	GDU	C1'-O3B-PB-O2B
3	A	602	GDU	O5'-C1'-O3B-PB
3	B	602	GDU	O4D-C4D-C5D-O5D
3	B	602	GDU	C5D-O5D-PA-O3A
3	B	602	GDU	PA-O3A-PB-O3B
3	B	602	GDU	C1'-O3B-PB-O2B
3	B	602	GDU	O5'-C1'-O3B-PB
3	C	602	GDU	O4D-C4D-C5D-O5D
3	C	602	GDU	C5D-O5D-PA-O3A
3	C	602	GDU	PA-O3A-PB-O3B
3	C	602	GDU	C1'-O3B-PB-O1B
3	C	602	GDU	C1'-O3B-PB-O2B
3	C	602	GDU	O5'-C1'-O3B-PB
3	D	602	GDU	C3D-C4D-C5D-O5D
3	D	602	GDU	O4D-C4D-C5D-O5D
3	D	602	GDU	C5D-O5D-PA-O3A
3	D	602	GDU	C1'-O3B-PB-O2B
3	D	602	GDU	O5'-C1'-O3B-PB
3	C	602	GDU	O5'-C5'-C6'-O6'
3	C	602	GDU	C3D-C4D-C5D-O5D
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C2'-C3'-C4'-C5'
3	D	602	GDU	C1'-O3B-PB-O3A
3	C	602	GDU	C4'-C5'-C6'-O6'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	D	601	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	B	602	GDU	C3D-C4D-C5D-O5D
2	C	601	FAD	O2'-C2'-C3'-C4'
3	A	602	GDU	O5'-C5'-C6'-O6'
2	B	601	FAD	O3'-C3'-C4'-C5'
3	D	602	GDU	O5'-C5'-C6'-O6'
3	C	602	GDU	C1'-O3B-PB-O3A
2	C	601	FAD	O2'-C2'-C3'-O3'
3	B	602	GDU	O5'-C5'-C6'-O6'
3	A	602	GDU	C2D-C1D-N1-C6
3	B	602	GDU	C1'-O3B-PB-O3A
2	A	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	C2'-C1'-N10-C9A
3	A	602	GDU	C1'-O3B-PB-O3A
2	B	601	FAD	C2'-C1'-N10-C10
2	A	601	FAD	C4'-C5'-O5'-P
2	D	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	P-O3P-PA-O5B
2	C	601	FAD	P-O3P-PA-O5B
2	D	601	FAD	P-O3P-PA-O5B
3	D	602	GDU	PA-O3A-PB-O3B
3	B	602	GDU	C2'-C1'-O3B-PB
3	C	602	GDU	C2'-C1'-O3B-PB
3	A	602	GDU	O4D-C1D-N1-C6
2	C	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	PA-O3P-P-O1P
3	D	602	GDU	C1'-O3B-PB-O1B
2	A	601	FAD	C5B-O5B-PA-O1A
3	A	602	GDU	C5D-O5D-PA-O1A
3	A	602	GDU	C5D-O5D-PA-O2A
3	B	602	GDU	C5D-O5D-PA-O1A
3	B	602	GDU	C5D-O5D-PA-O2A
3	C	602	GDU	C5D-O5D-PA-O1A
3	C	602	GDU	C5D-O5D-PA-O2A
3	D	602	GDU	C5D-O5D-PA-O1A
3	D	602	GDU	C5D-O5D-PA-O2A
2	B	601	FAD	C1'-C2'-C3'-O3'
3	A	602	GDU	C2D-C1D-N1-C2
3	A	602	GDU	O4D-C1D-N1-C2
2	A	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C5'-O5'-P-O3P
2	D	601	FAD	C5B-O5B-PA-O3P
3	A	602	GDU	C1'-O3B-PB-O1B
3	B	602	GDU	C1'-O3B-PB-O1B
2	D	601	FAD	O4'-C4'-C5'-O5'

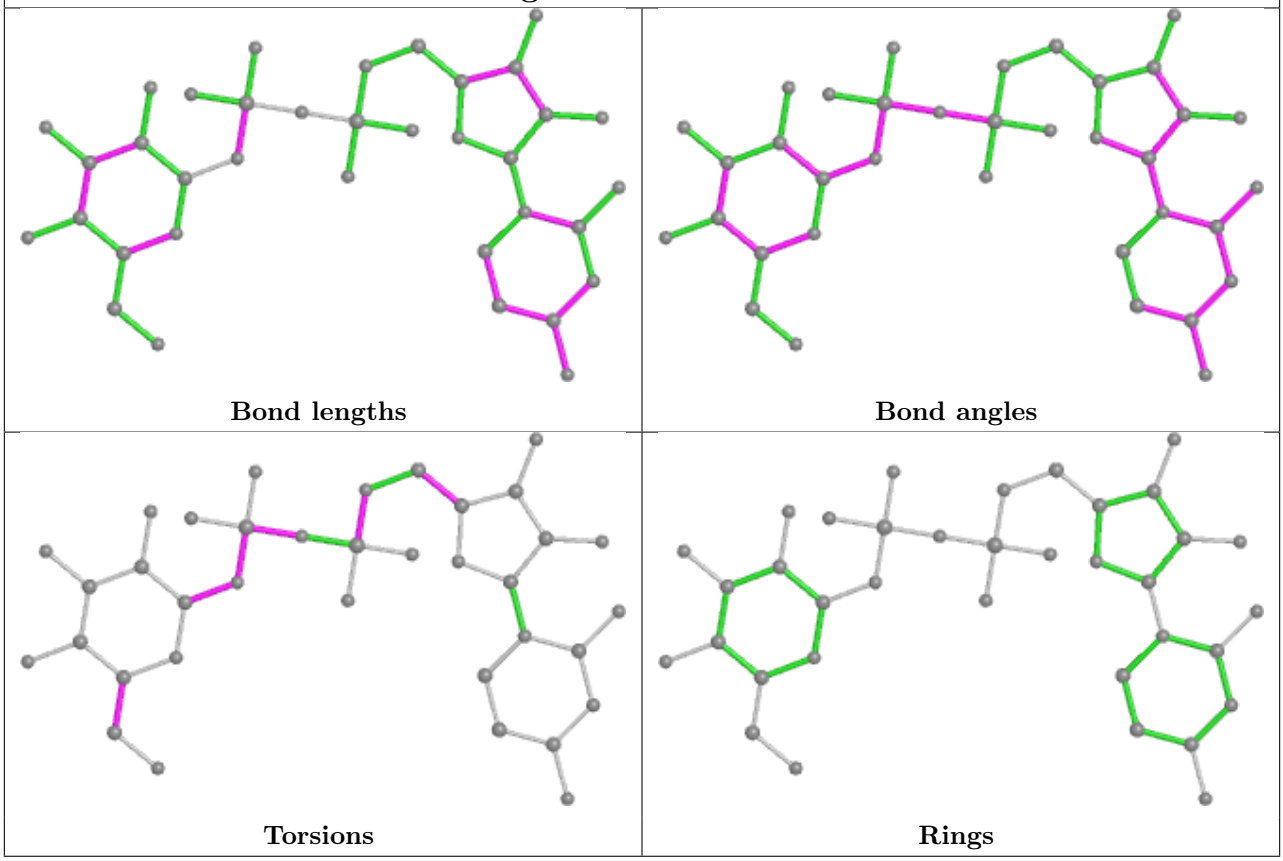
There are no ring outliers.

5 monomers are involved in 11 short contacts:

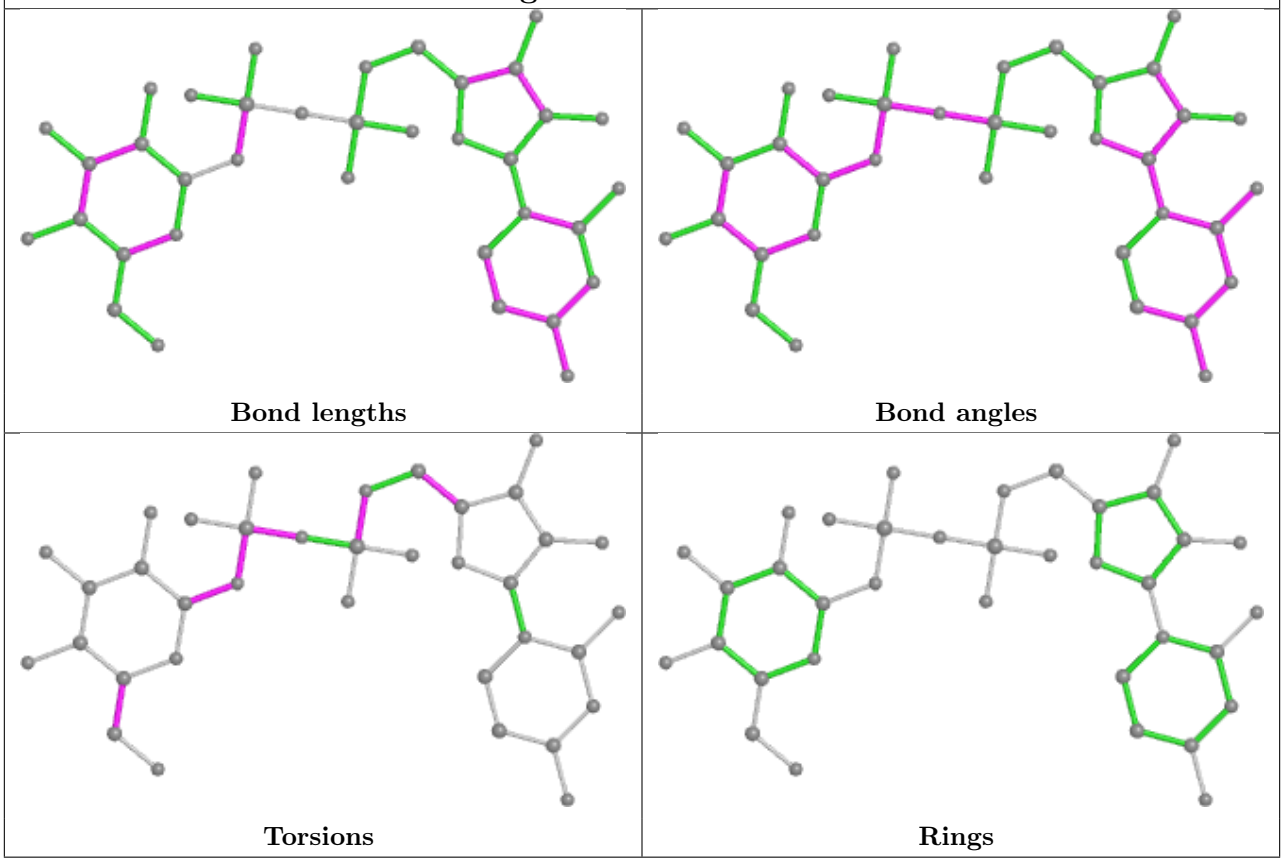
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	GDU	5	0
3	D	602	GDU	2	0
3	B	602	GDU	2	0
2	D	601	FAD	1	0
3	A	602	GDU	1	0

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 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 GDU C 602



Ligand GDU D 602



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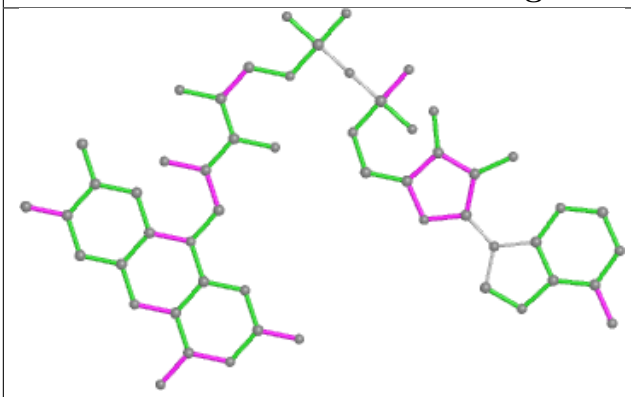
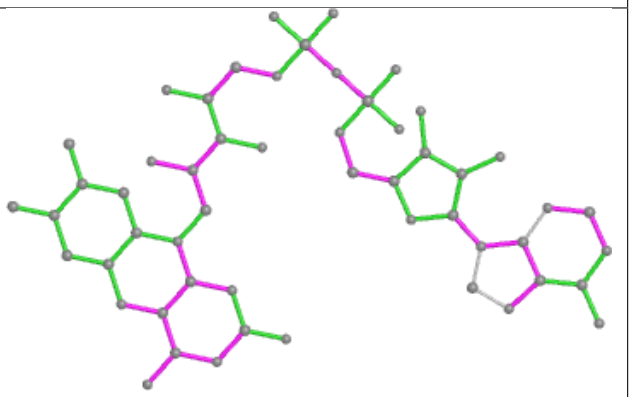
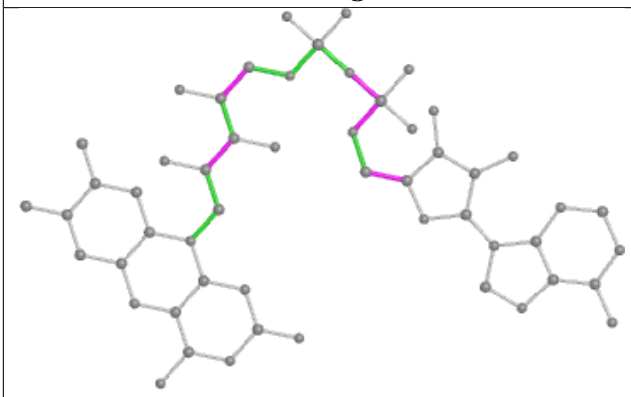


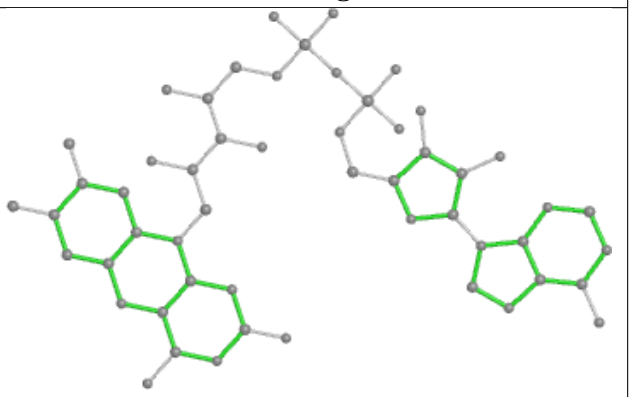
Bond lengths



Bond angles

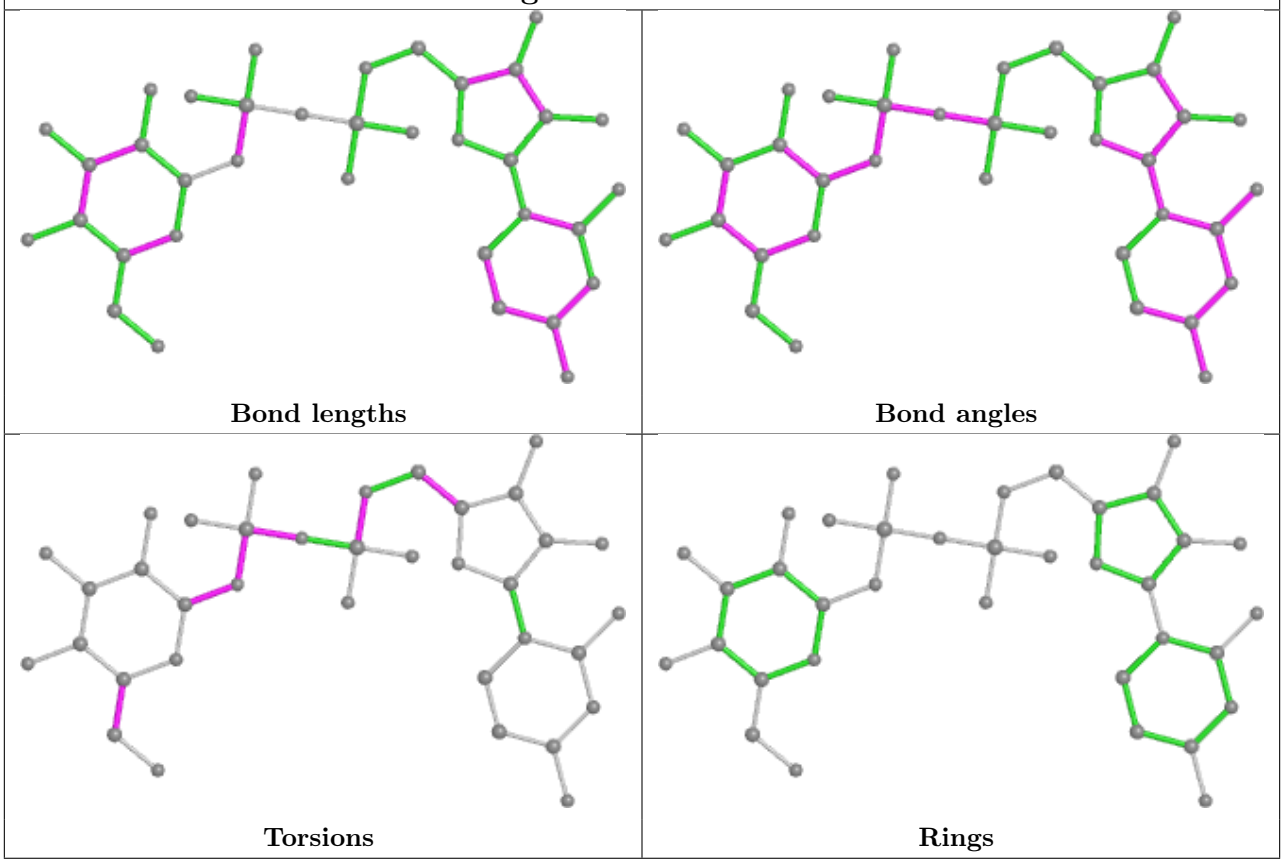


Torsions

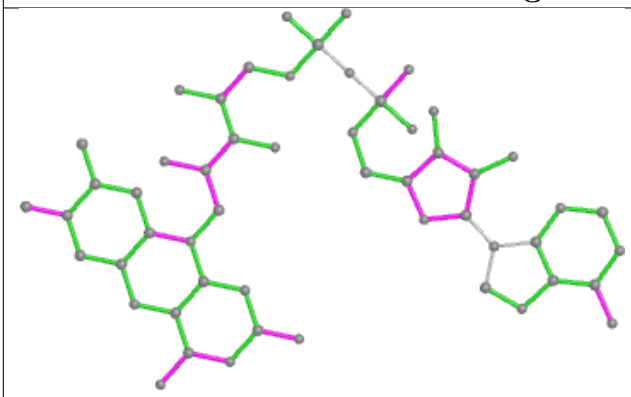


Rings

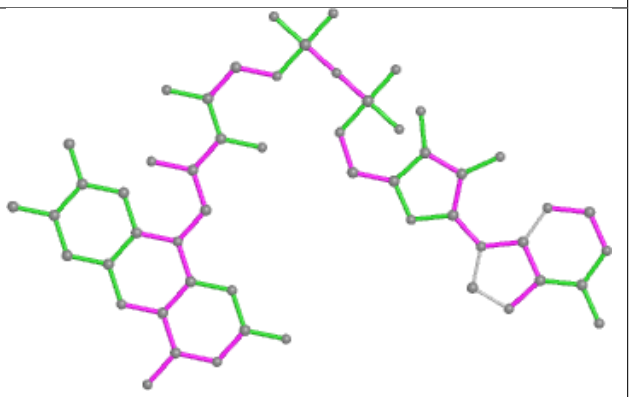
Ligand GDU B 602



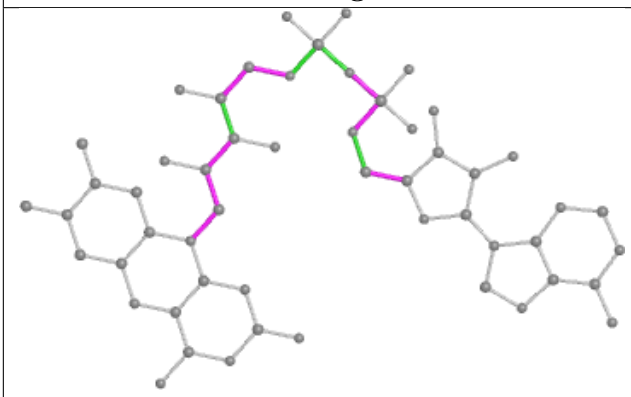
Ligand FAD D 601



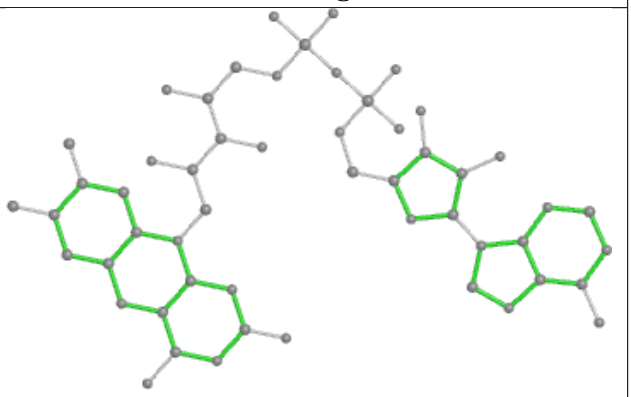
Bond lengths



Bond angles

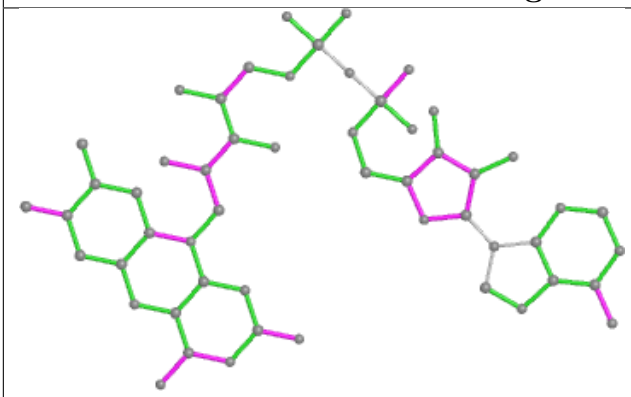


Torsions

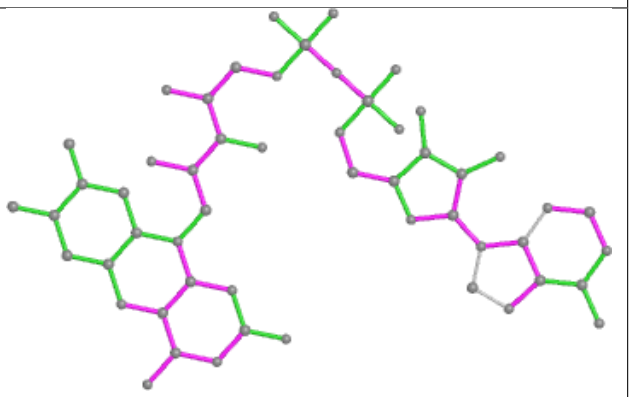


Rings

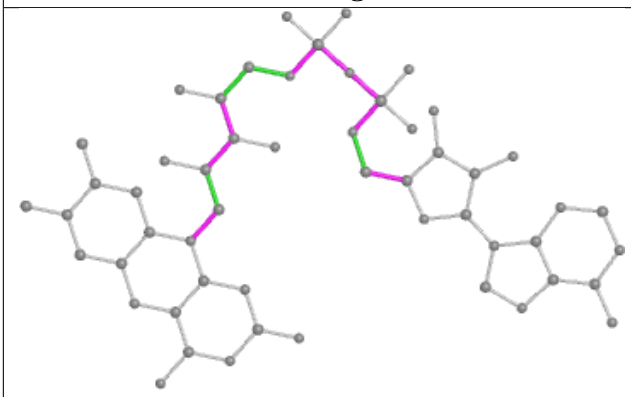
Ligand FAD B 601



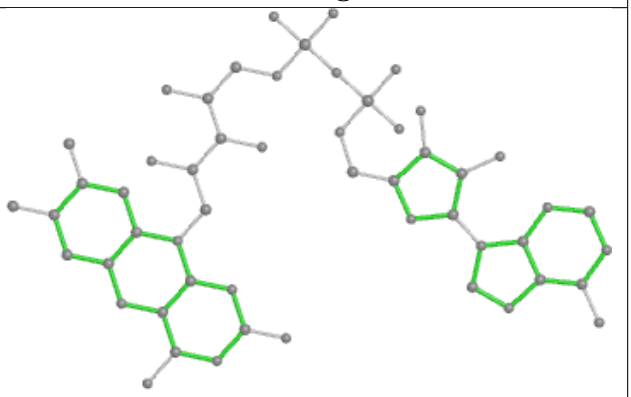
Bond lengths



Bond angles

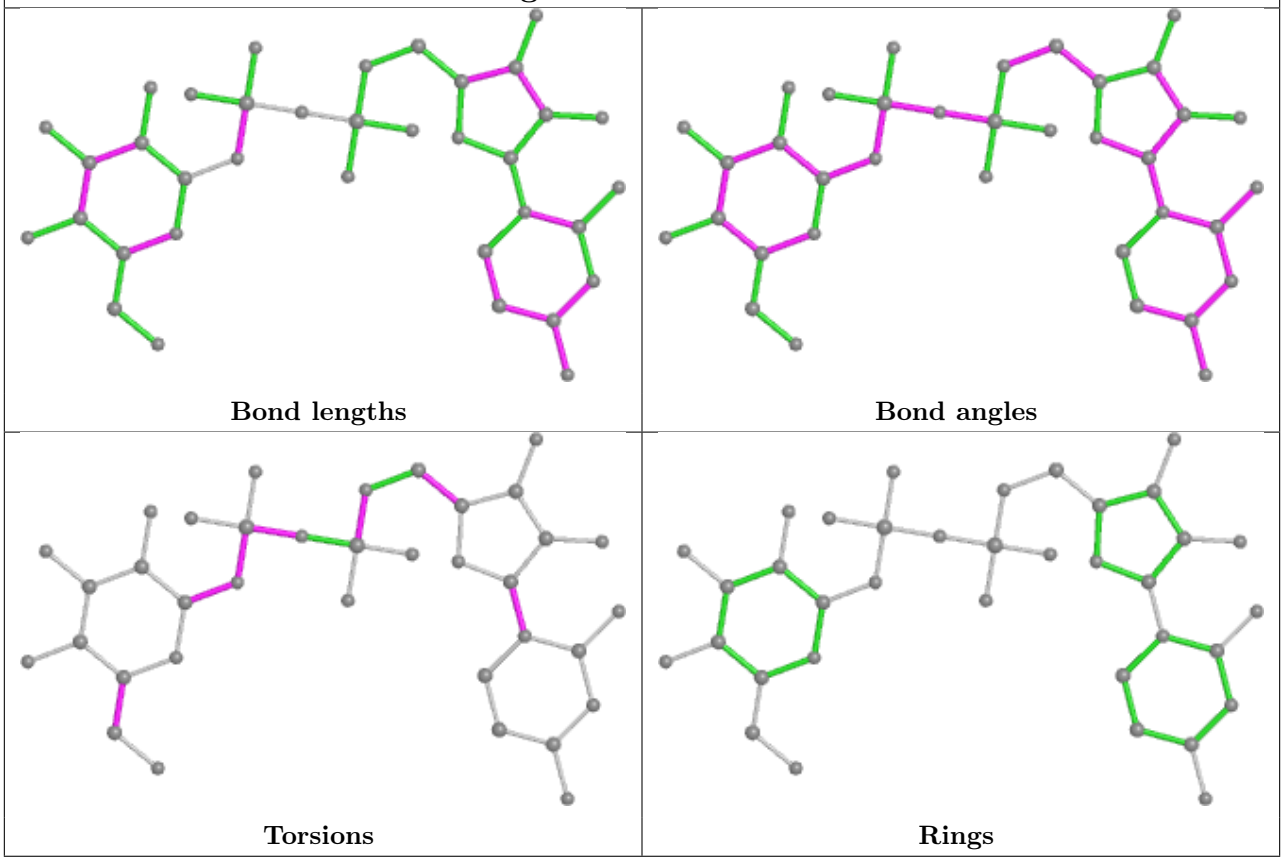


Torsions

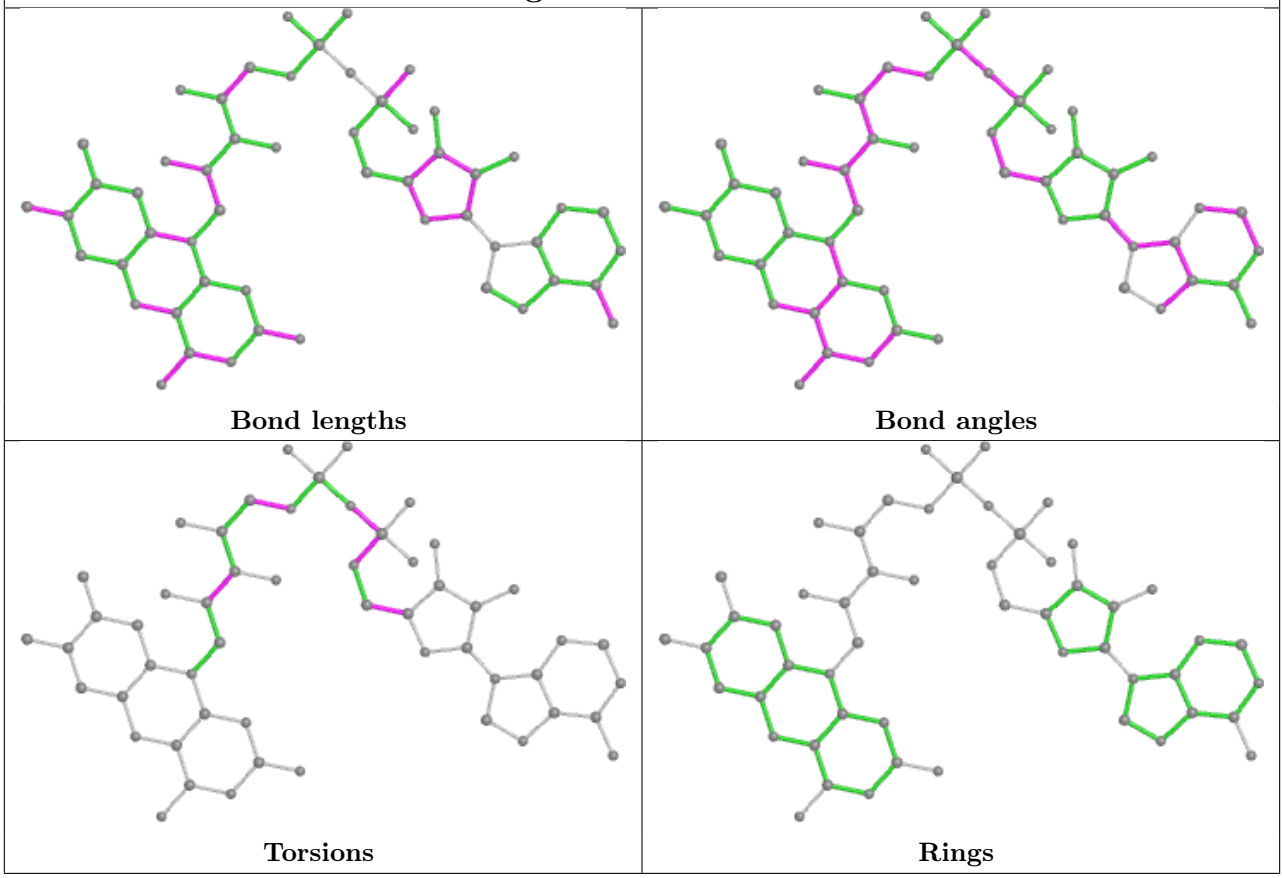


Rings

Ligand GDU A 602



Ligand FAD A 601



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	510/510 (100%)	0.31	28 (5%)	25	13	37, 64, 98, 145	1 (0%)
1	B	510/510 (100%)	0.31	18 (3%)	44	27	36, 63, 97, 144	2 (0%)
1	C	510/510 (100%)	0.27	19 (3%)	41	25	35, 63, 99, 146	5 (0%)
1	D	510/510 (100%)	0.43	33 (6%)	18	10	37, 65, 99, 146	5 (0%)
All	All	2040/2040 (100%)	0.33	98 (4%)	30	17	35, 64, 99, 146	13 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	ALA	5.0
1	B	358	GLN	4.9
1	D	255	GLN	4.8
1	A	358	GLN	4.7
1	D	206	PRO	4.6
1	A	359	SER	4.4
1	C	203	ASN	4.4
1	D	207	ASN	4.4
1	D	341	GLU	4.3
1	D	205	GLY	4.2
1	C	204	TRP	4.0
1	C	184	ALA	4.0
1	A	2	THR	3.9
1	A	511	LEU	3.9
1	C	206	PRO	3.7
1	A	510	GLN	3.7
1	B	123	ASP	3.7
1	A	356	ARG	3.7
1	D	185	ALA	3.4
1	B	202	GLY	3.4
1	D	201	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	116	GLU	3.1
1	B	115	LYS	3.1
1	B	359	SER	3.1
1	B	341	GLU	3.0
1	A	205	GLY	3.0
1	B	157	LEU	3.0
1	B	201	ALA	2.9
1	D	505	ALA	2.9
1	B	282	GLU	2.9
1	B	510	GLN	2.9
1	C	84	ASP	2.9
1	A	355	SER	2.9
1	A	341	GLU	2.9
1	D	510	GLN	2.8
1	A	357	PRO	2.8
1	A	361	GLU	2.8
1	D	506	LYS	2.8
1	D	258	THR	2.8
1	C	205	GLY	2.8
1	A	185	ALA	2.8
1	A	352	ALA	2.8
1	A	184	ALA	2.7
1	C	510	GLN	2.7
1	D	180	GLY	2.7
1	C	192	THR	2.7
1	D	509	ALA	2.6
1	B	205	GLY	2.6
1	A	508	LYS	2.6
1	D	200	THR	2.6
1	D	342	ALA	2.5
1	A	200	THR	2.5
1	D	276	GLU	2.5
1	D	365	GLY	2.5
1	D	243	THR	2.5
1	A	201	ALA	2.5
1	D	208	ALA	2.5
1	C	186	PRO	2.5
1	D	204	TRP	2.4
1	A	346	LEU	2.4
1	B	204	TRP	2.4
1	A	203	ASN	2.4
1	D	508	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	238	GLU	2.3
1	A	347	PRO	2.3
1	B	511	LEU	2.3
1	A	259	THR	2.3
1	D	279	ASN	2.3
1	D	121	CYS	2.3
1	B	119	VAL	2.3
1	D	186	PRO	2.3
1	D	259	THR	2.3
1	A	3	HIS	2.2
1	A	115	LYS	2.2
1	C	308	GLU	2.2
1	A	204	TRP	2.2
1	D	3	HIS	2.2
1	A	123	ASP	2.2
1	D	401	LEU	2.2
1	D	308	GLU	2.2
1	D	305	SER	2.2
1	B	134	VAL	2.2
1	C	198	GLY	2.1
1	D	511	LEU	2.1
1	C	185	ALA	2.1
1	C	200	THR	2.1
1	D	301	GLY	2.1
1	A	360	THR	2.1
1	A	207	ASN	2.1
1	C	2	THR	2.1
1	D	366	PRO	2.1
1	C	202	GLY	2.0
1	C	207	ASN	2.0
1	B	343	SER	2.0
1	C	499	ASP	2.0
1	B	281	GLN	2.0
1	A	202	GLY	2.0
1	C	136	ASN	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)

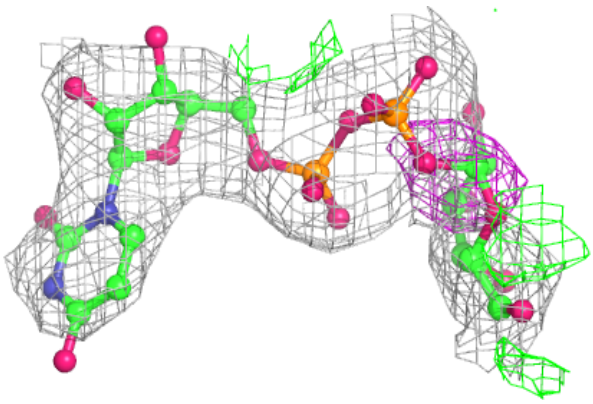
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

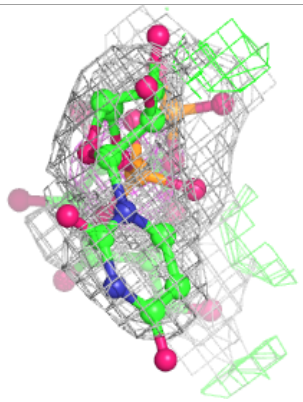
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GDU	B	602	36/36	0.86	0.28	75,104,146,148	0
3	GDU	C	602	36/36	0.86	0.26	77,116,139,156	0
3	GDU	D	602	36/36	0.86	0.29	78,117,137,144	0
3	GDU	A	602	36/36	0.88	0.25	79,101,136,148	0
2	FAD	D	601	53/53	0.92	0.27	34,66,76,99	0
2	FAD	C	601	53/53	0.95	0.24	37,53,68,80	0
2	FAD	A	601	53/53	0.95	0.23	31,51,69,78	0
2	FAD	B	601	53/53	0.95	0.26	32,55,66,80	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 GDU B 602:

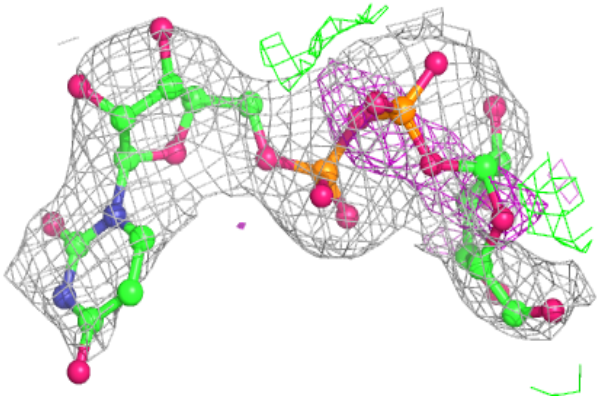
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

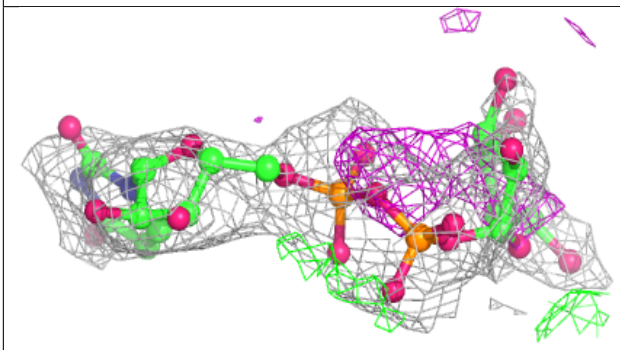


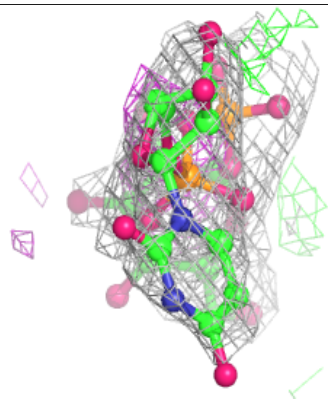


Electron density around GDU C 602:

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

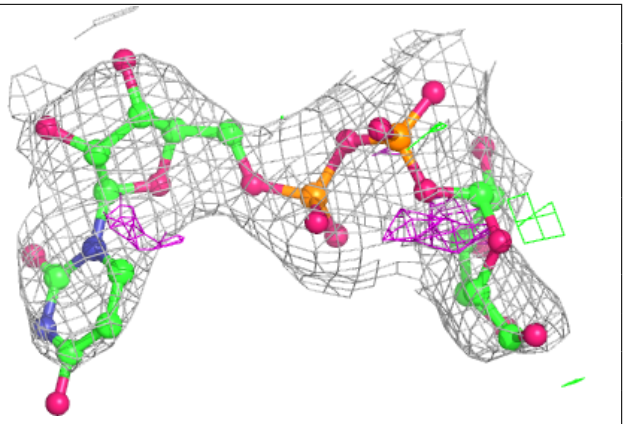


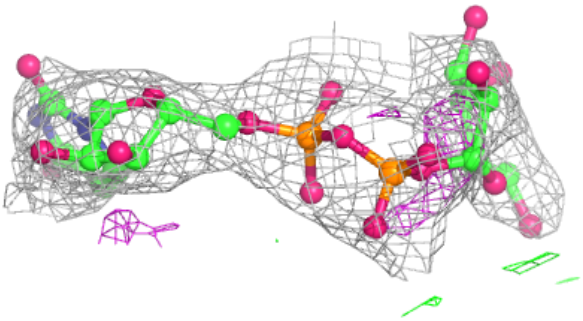


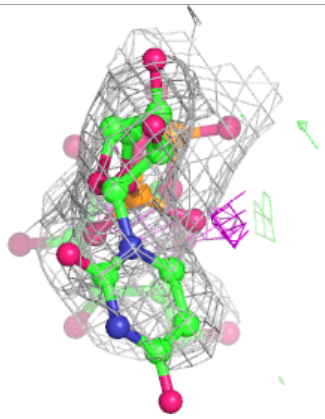


Electron density around GDU D 602:

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







Electron density around GDU A 602:

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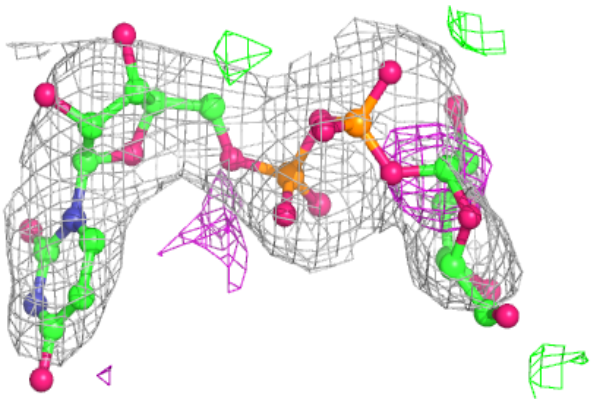
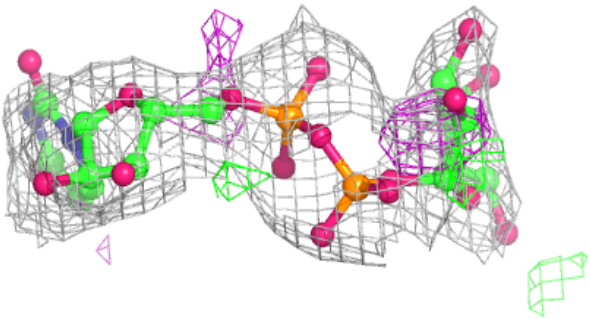
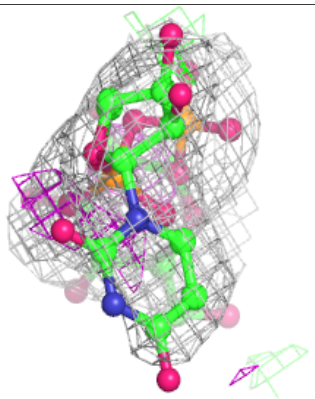
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

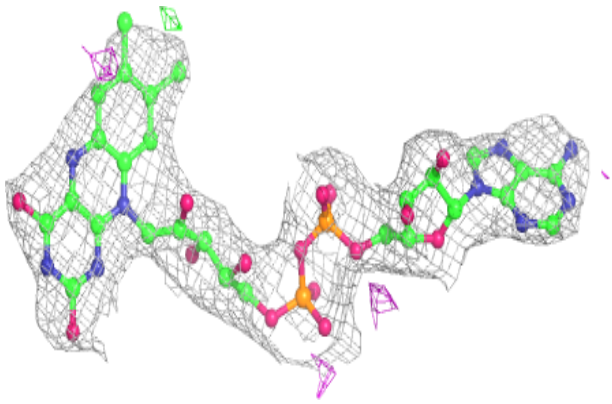


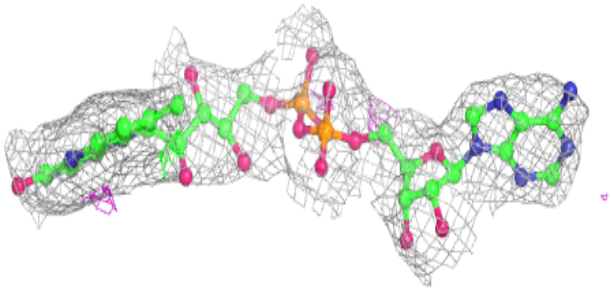


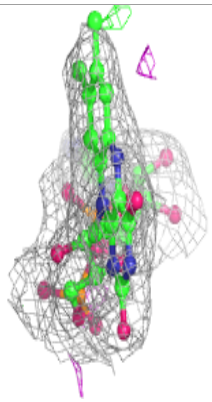


Electron density around FAD D 601:

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

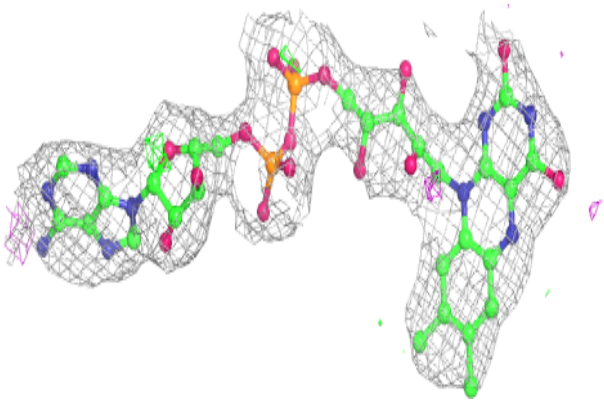


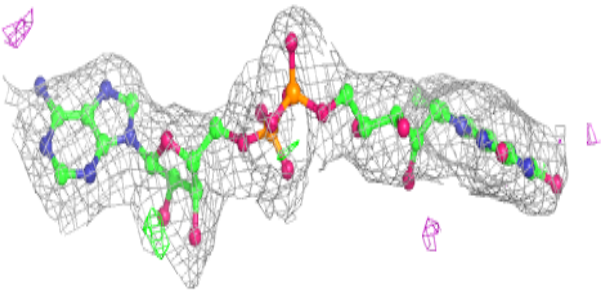


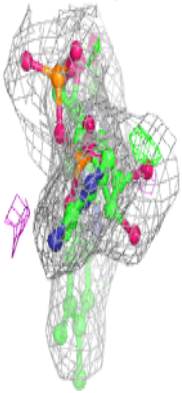


Electron density around FAD C 601:

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

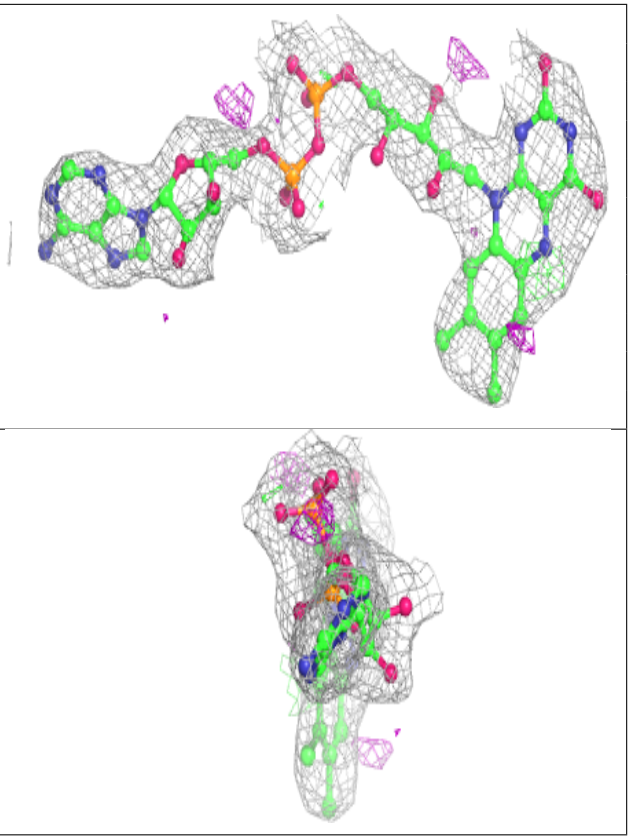






Electron density around FAD A 601:

$2mF_o$-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 601:

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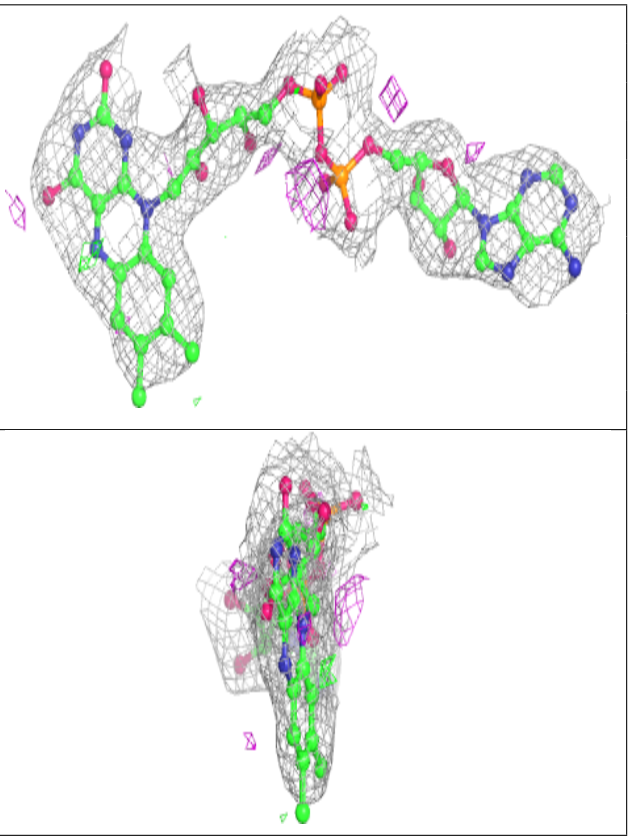
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.