



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:24 pm BST

PDB ID : 4NCR
Title : Crystal structure of M. tuberculosis DprE1 in complex with PBTZ169
Authors : Neres, J.; Pojer, F.; Cole, S.T.
Deposited on : 2013-10-25
Resolution : 1.88 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

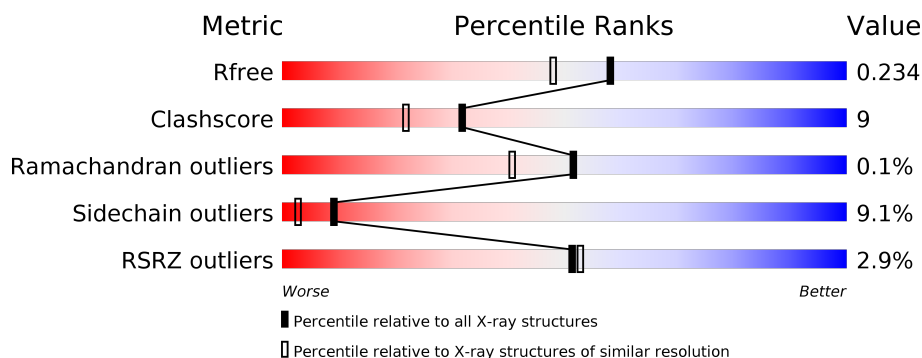
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	481	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6907 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 decaprenylphosphoryl-beta-D-ribose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3286	2085	581	610	10			
1	B	413	Total	C	N	O	S	0	0	0
			3173	2012	563	588	10			

There are 40 discrepancies between the modelled and reference sequences:

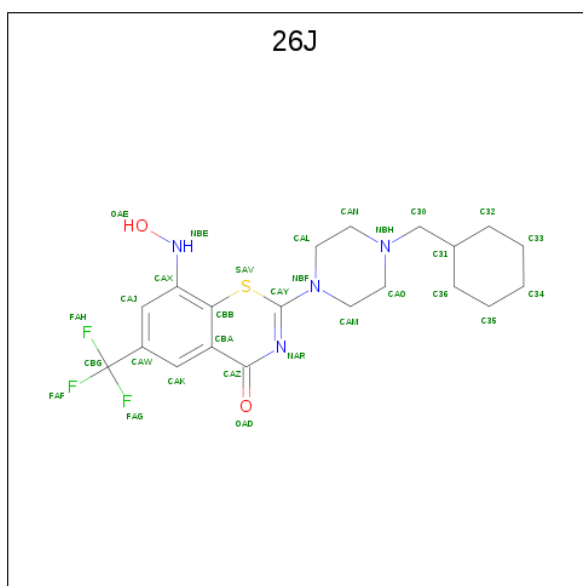
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P72056
A	-18	GLY	-	EXPRESSION TAG	UNP P72056
A	-17	SER	-	EXPRESSION TAG	UNP P72056
A	-16	SER	-	EXPRESSION TAG	UNP P72056
A	-15	HIS	-	EXPRESSION TAG	UNP P72056
A	-14	HIS	-	EXPRESSION TAG	UNP P72056
A	-13	HIS	-	EXPRESSION TAG	UNP P72056
A	-12	HIS	-	EXPRESSION TAG	UNP P72056
A	-11	HIS	-	EXPRESSION TAG	UNP P72056
A	-10	HIS	-	EXPRESSION TAG	UNP P72056
A	-9	SER	-	EXPRESSION TAG	UNP P72056
A	-8	SER	-	EXPRESSION TAG	UNP P72056
A	-7	GLY	-	EXPRESSION TAG	UNP P72056
A	-6	LEU	-	EXPRESSION TAG	UNP P72056
A	-5	VAL	-	EXPRESSION TAG	UNP P72056
A	-4	PRO	-	EXPRESSION TAG	UNP P72056
A	-3	ARG	-	EXPRESSION TAG	UNP P72056
A	-2	GLY	-	EXPRESSION TAG	UNP P72056
A	-1	SER	-	EXPRESSION TAG	UNP P72056
A	0	HIS	-	EXPRESSION TAG	UNP P72056
B	-19	MET	-	EXPRESSION TAG	UNP P72056
B	-18	GLY	-	EXPRESSION TAG	UNP P72056
B	-17	SER	-	EXPRESSION TAG	UNP P72056
B	-16	SER	-	EXPRESSION TAG	UNP P72056
B	-15	HIS	-	EXPRESSION TAG	UNP P72056

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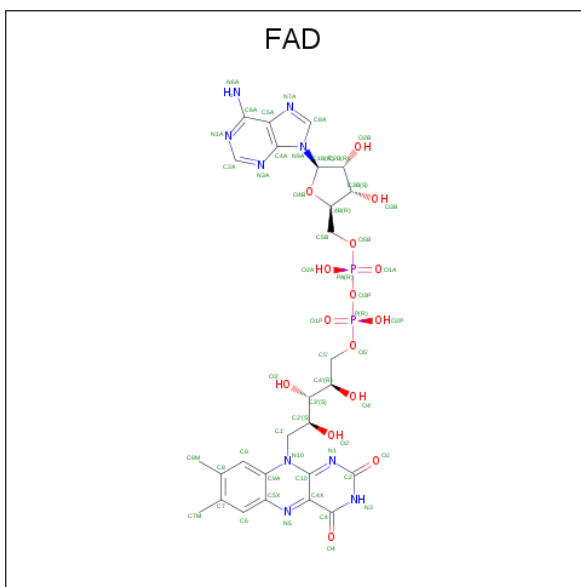
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP P72056
B	-13	HIS	-	EXPRESSION TAG	UNP P72056
B	-12	HIS	-	EXPRESSION TAG	UNP P72056
B	-11	HIS	-	EXPRESSION TAG	UNP P72056
B	-10	HIS	-	EXPRESSION TAG	UNP P72056
B	-9	SER	-	EXPRESSION TAG	UNP P72056
B	-8	SER	-	EXPRESSION TAG	UNP P72056
B	-7	GLY	-	EXPRESSION TAG	UNP P72056
B	-6	LEU	-	EXPRESSION TAG	UNP P72056
B	-5	VAL	-	EXPRESSION TAG	UNP P72056
B	-4	PRO	-	EXPRESSION TAG	UNP P72056
B	-3	ARG	-	EXPRESSION TAG	UNP P72056
B	-2	GLY	-	EXPRESSION TAG	UNP P72056
B	-1	SER	-	EXPRESSION TAG	UNP P72056
B	0	HIS	-	EXPRESSION TAG	UNP P72056

- Molecule 2 is 2-(4-(cyclohexylmethyl)piperazin-1-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one, bound form (three-letter code: 26J) (formula: C₂₀H₂₅F₃N₄O₂S).



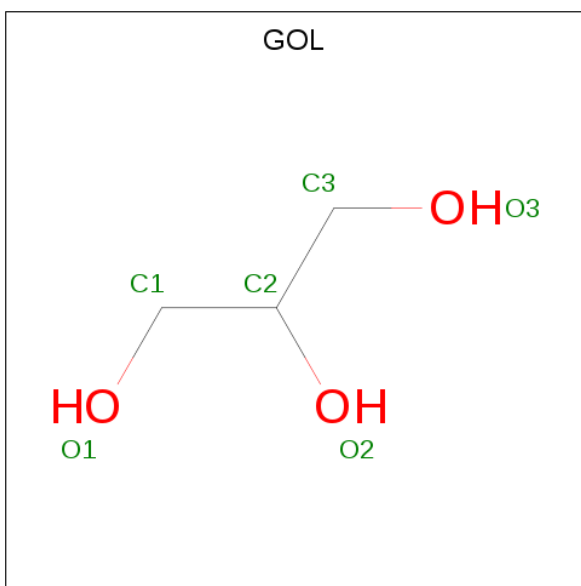
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			30	20	3	4	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			30	20	3	4	2	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



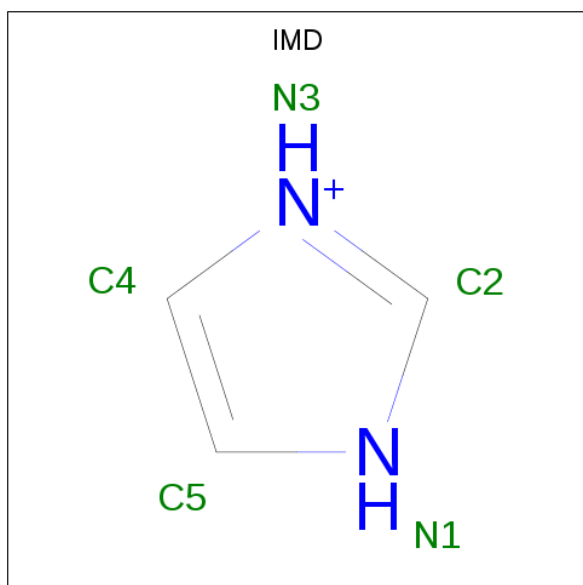
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			5	3	2		

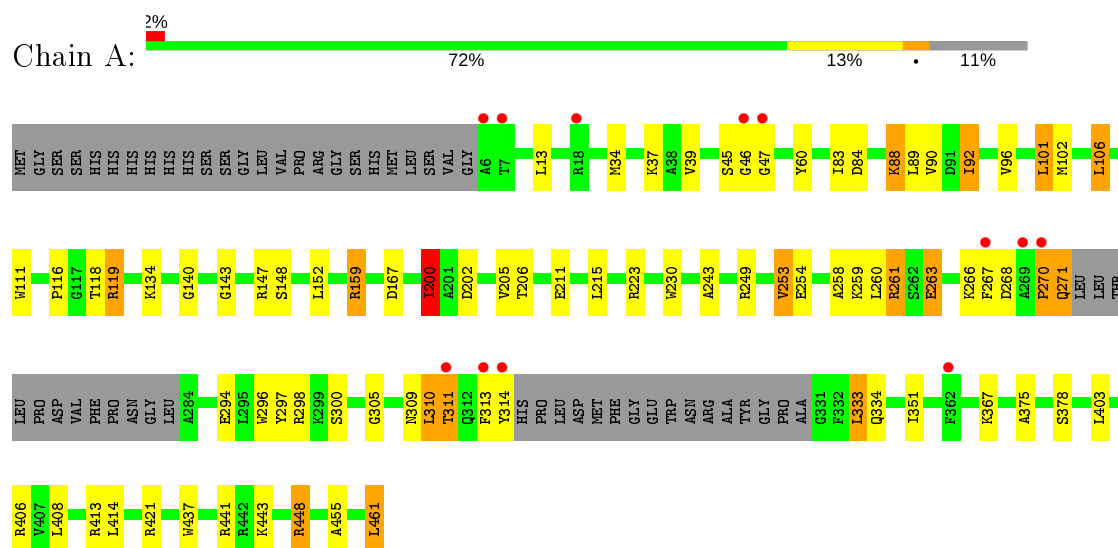
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	150	Total	O	0	0
			150	150		
6	B	103	Total	O	0	0
			103	103		

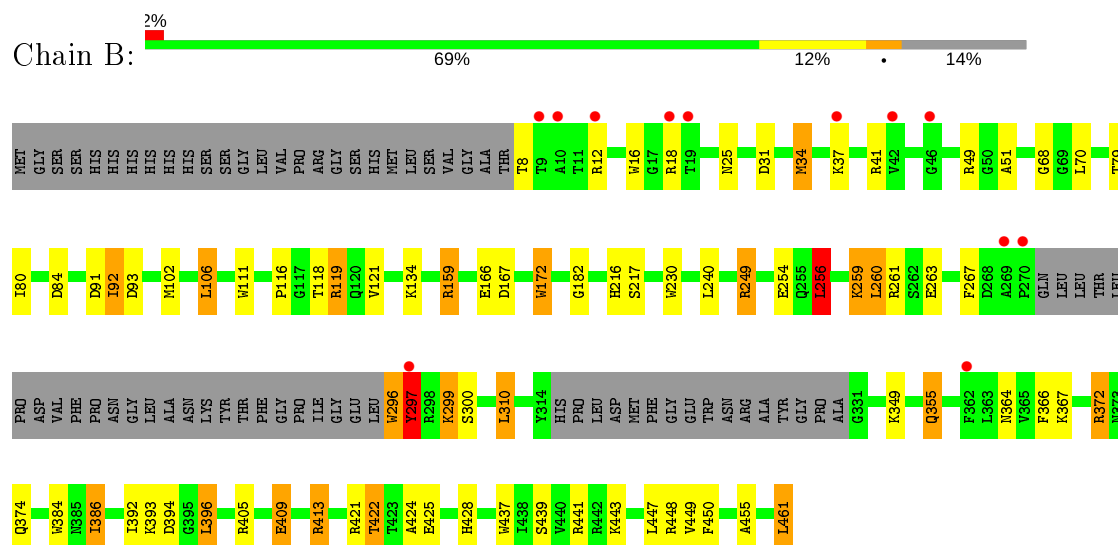
3 Residue-property plots [i](#)

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: decaprenylphosphoryl-beta-D-ribose oxidase



- Molecule 1: decaprenylphosphoryl-beta-D-ribose oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.05Å 85.00Å 81.37Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	48.87 – 1.88 48.87 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.87-1.88) 98.0 (48.87-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.234 0.186 , 0.234	Depositor DCC
R_{free} test set	3919 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6907	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IMD, FAD, 26J

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	1.18	8/3360 (0.2%)	1.13	11/4559 (0.2%)
1	B	1.10	9/3244 (0.3%)	1.10	14/4401 (0.3%)
All	All	1.14	17/6604 (0.3%)	1.11	25/8960 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	TYR	CZ-OH	12.04	1.58	1.37
1	B	437	TRP	CD2-CE2	6.24	1.48	1.41
1	B	111	TRP	CD2-CE2	6.16	1.48	1.41
1	A	140	GLY	N-CA	-6.05	1.36	1.46
1	A	230	TRP	CD2-CE2	5.98	1.48	1.41
1	B	409	GLU	CG-CD	-5.78	1.43	1.51
1	B	384	TRP	CD2-CE2	5.62	1.48	1.41
1	A	143	GLY	N-CA	5.62	1.54	1.46
1	A	111	TRP	CD2-CE2	5.53	1.48	1.41
1	B	230	TRP	CD2-CE2	5.53	1.48	1.41
1	B	297	TYR	CE2-CZ	5.47	1.45	1.38
1	A	243	ALA	C-O	5.37	1.33	1.23
1	A	437	TRP	CD2-CE2	5.34	1.47	1.41
1	B	16	TRP	CD2-CE2	5.26	1.47	1.41
1	A	148	SER	CA-CB	5.18	1.60	1.52
1	B	172	TRP	CD2-CE2	5.13	1.47	1.41
1	A	296	TRP	CD2-CE2	5.05	1.47	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	B	413	ARG	NE-CZ-NH2	-8.34	116.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	LEU	CB-CG-CD2	-8.28	96.92	111.00
1	A	223	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	106	LEU	CB-CG-CD2	6.84	122.62	111.00
1	A	223	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	372	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	159	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	372	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	101	LEU	CB-CG-CD2	6.08	121.33	111.00
1	B	310	LEU	CA-CB-CG	-5.96	101.59	115.30
1	B	93	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	414	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	A	106	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	B	405	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	A	147	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	249	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	91	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	409	GLU	CG-CD-OE2	-5.34	107.61	118.30
1	A	200	ILE	CB-CA-C	-5.25	101.10	111.60
1	A	408	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	B	256	LEU	CB-CG-CD1	5.11	119.69	111.00
1	B	134	LYS	CD-CE-NZ	-5.10	99.97	111.70
1	B	93	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	202	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3286	0	3261	59	0
1	B	3173	0	3151	54	0
2	A	30	0	24	3	0
2	B	30	0	24	1	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	0	24	2	0
4	B	6	0	8	3	0
5	B	5	0	5	2	0
6	A	150	0	0	5	0
6	B	103	0	0	3	0
All	All	6907	0	6559	117	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 9.

All (117) 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:119:ARG:HH11	1:A:119:ARG:HG3	1.10	1.09
1:B:119:ARG:HG3	1:B:119:ARG:HH11	1.16	1.09
1:A:102:MET:HE1	1:A:119:ARG:HD3	1.43	1.01
1:A:448:ARG:CG	1:A:448:ARG:HH11	1.75	0.99
1:B:159:ARG:HH11	1:B:159:ARG:HG2	1.27	0.98
1:A:102:MET:HE1	1:A:119:ARG:CD	1.94	0.98
1:A:102:MET:CE	1:A:119:ARG:HD2	1.98	0.94
1:A:271:GLN:HG2	1:A:271:GLN:O	1.70	0.92
1:A:102:MET:HE3	1:A:119:ARG:HD2	1.51	0.90
1:B:79:THR:HA	4:B:503:GOL:H32	1.50	0.90
1:A:102:MET:CE	1:A:119:ARG:CD	2.49	0.89
1:A:309:ASN:OD1	1:A:311:THR:HG23	1.72	0.88
1:B:299:LYS:HG3	1:B:300:SER:N	1.89	0.87
1:B:296:TRP:HE3	1:B:297:TYR:H	1.24	0.84
1:B:102:MET:HE1	1:B:119:ARG:HD3	1.67	0.77
1:B:299:LYS:HG3	1:B:300:SER:H	1.50	0.76
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.49	0.76
1:A:448:ARG:HH11	1:A:448:ARG:HG3	1.51	0.75
1:B:119:ARG:CG	1:B:119:ARG:HH11	1.96	0.75
1:B:159:ARG:CG	1:B:159:ARG:HH11	2.00	0.74
1:B:102:MET:HE1	1:B:119:ARG:CD	2.19	0.73
2:A:501:26J:OAE	2:A:501:26J:SAV	2.47	0.72
1:A:448:ARG:CG	1:A:448:ARG:NH1	2.45	0.70
1:B:166:GLU:O	1:B:167:ASP:HB2	1.89	0.70
1:A:119:ARG:NH1	1:A:119:ARG:HG3	1.88	0.70
1:B:119:ARG:HG3	1:B:119:ARG:NH1	1.92	0.68
1:A:84:ASP:OD2	5:B:504:IMD:H2	1.94	0.68
1:A:102:MET:HG2	1:A:267:PHE:CZ	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:O	1:A:311:THR:HG21	1.96	0.66
1:A:448:ARG:HG2	1:A:448:ARG:NH1	2.08	0.64
1:A:270:PRO:HB3	1:A:271:GLN:HA	1.81	0.63
1:B:102:MET:CE	1:B:119:ARG:HD2	2.28	0.63
1:B:240:LEU:HD22	1:B:355:GLN:HG3	1.81	0.63
1:A:258:ALA:HA	1:A:261:ARG:HH21	1.62	0.63
1:B:259:LYS:H	1:B:259:LYS:CE	2.12	0.62
1:B:249:ARG:HD2	6:B:674:HOH:O	1.99	0.62
1:A:375:ALA:HB3	1:A:378:SER:HB2	1.80	0.62
1:B:159:ARG:NH1	1:B:159:ARG:HG2	2.05	0.61
1:A:455:ALA:HB1	1:A:461:LEU:HD13	1.83	0.60
1:A:102:MET:HG2	1:A:267:PHE:HZ	1.64	0.60
2:B:501:26J:SAV	2:B:501:26J:OAE	2.57	0.60
1:B:259:LYS:H	1:B:259:LYS:HE2	1.66	0.59
1:B:102:MET:CE	1:B:119:ARG:CD	2.79	0.59
1:B:80:ILE:H	4:B:503:GOL:C3	2.15	0.59
1:A:270:PRO:CB	1:A:271:GLN:HA	2.32	0.59
1:A:271:GLN:CG	1:A:271:GLN:O	2.49	0.58
1:A:249:ARG:NH2	6:A:702:HOH:O	2.35	0.58
1:B:31:ASP:HB3	1:B:34:MET:HG3	1.86	0.57
1:B:424:ALA:O	1:B:428:HIS:CD2	2.57	0.57
1:A:215:LEU:C	1:A:215:LEU:HD23	2.24	0.57
1:B:80:ILE:H	4:B:503:GOL:H32	1.69	0.57
1:A:200:ILE:HG22	1:A:305:GLY:HA2	1.87	0.56
1:A:333:LEU:HD23	1:A:421:ARG:CZ	2.35	0.56
1:B:102:MET:HG2	1:B:267:PHE:CZ	2.42	0.55
2:A:501:26J:H17	2:A:501:26J:H11	1.89	0.54
1:B:102:MET:HE3	1:B:119:ARG:HD2	1.88	0.54
1:B:374:GLN:HG2	6:B:635:HOH:O	2.06	0.54
1:A:441:ARG:NH2	1:A:461:LEU:HD12	2.23	0.54
1:B:92:ILE:H	1:B:92:ILE:HD13	1.73	0.54
1:A:310:LEU:HD11	1:A:314:TYR:HE2	1.72	0.53
1:A:253:VAL:HG23	1:A:261:ARG:HG3	1.91	0.53
1:A:116:PRO:HG2	1:A:118:THR:O	2.09	0.53
1:A:102:MET:HG3	6:A:614:HOH:O	2.09	0.53
1:A:60:TYR:CE2	1:A:334:GLN:HG2	2.44	0.52
1:B:296:TRP:HE3	1:B:297:TYR:N	2.00	0.52
1:B:310:LEU:O	1:B:310:LEU:HG	2.04	0.52
1:B:102:MET:HG2	1:B:267:PHE:CE2	2.46	0.51
1:A:333:LEU:CD2	1:A:421:ARG:CZ	2.89	0.51
1:B:49:ARG:HG3	1:B:68:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:HG21	1:A:298:ARG:HA	1.94	0.50
1:A:206:THR:HB	1:A:211:GLU:HB3	1.94	0.50
1:B:256:LEU:O	1:B:261:ARG:HD2	2.11	0.50
1:B:116:PRO:HG2	1:B:118:THR:O	2.13	0.49
1:A:46:GLY:HA2	1:A:47:GLY:HA2	1.58	0.48
1:B:182:GLY:HA2	1:B:450:PHE:CE2	2.49	0.48
1:A:441:ARG:HH21	1:A:461:LEU:HD12	1.77	0.47
1:B:84:ASP:OD2	5:B:504:IMD:H5	2.14	0.47
1:A:258:ALA:CA	1:A:261:ARG:HH21	2.25	0.47
1:A:102:MET:HE3	1:A:119:ARG:CD	2.26	0.47
1:A:89:LEU:HD12	4:A:504:GOL:H31	1.98	0.46
1:B:172:TRP:CD2	1:B:374:GLN:HG3	2.49	0.46
1:B:393:LYS:O	1:B:396:LEU:HB2	2.16	0.46
1:A:83:ILE:HG23	1:A:90:VAL:HG12	1.98	0.46
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.81	0.46
1:B:424:ALA:O	1:B:428:HIS:HD2	1.99	0.45
1:A:119:ARG:NH1	6:A:640:HOH:O	2.48	0.45
1:A:106:LEU:HD12	1:A:267:PHE:CE2	2.52	0.45
1:B:51:ALA:N	1:B:449:VAL:O	2.42	0.45
1:B:25:ASN:O	1:B:70:LEU:HD12	2.16	0.45
1:A:88:LYS:HE3	1:A:88:LYS:HB2	1.57	0.45
2:A:501:26J:H11	2:A:501:26J:C32	2.47	0.45
1:A:258:ALA:HA	1:A:261:ARG:HD3	1.99	0.44
1:B:119:ARG:NH1	6:B:637:HOH:O	2.50	0.44
1:B:441:ARG:NH2	1:B:461:LEU:HD12	2.33	0.44
1:A:297:TYR:OH	4:A:503:GOL:H12	2.17	0.44
1:B:254:GLU:H	1:B:254:GLU:CD	2.20	0.44
1:A:92:ILE:HB	1:A:96:VAL:HG21	2.01	0.43
1:B:37:LYS:HA	1:B:37:LYS:HD2	1.72	0.43
1:A:443:LYS:HE2	6:A:742:HOH:O	2.19	0.43
1:B:172:TRP:CE2	1:B:374:GLN:HG3	2.53	0.43
1:B:259:LYS:HE2	1:B:259:LYS:HB2	1.46	0.43
1:A:102:MET:CG	1:A:267:PHE:HZ	2.30	0.42
1:B:455:ALA:HB1	1:B:461:LEU:HD13	2.02	0.42
1:B:92:ILE:N	1:B:92:ILE:HD13	2.35	0.42
1:A:313:PHE:N	1:A:313:PHE:CD1	2.88	0.42
1:A:403:LEU:HD23	1:A:403:LEU:HA	1.75	0.42
1:A:134:LYS:HD3	6:A:699:HOH:O	2.20	0.42
1:A:254:GLU:H	1:A:254:GLU:CD	2.23	0.41
1:A:351:ILE:HA	1:A:351:ILE:HD13	1.93	0.41
1:A:263:GLU:HG2	1:A:266:LYS:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASN:HB3	1:B:386:ILE:HD11	2.03	0.41
1:B:421:ARG:HG2	1:B:422:THR:N	2.36	0.41
1:A:200:ILE:H	1:A:200:ILE:HD12	1.85	0.41
1:A:39:VAL:HG21	1:A:152:LEU:HD21	2.03	0.40
1:B:296:TRP:O	1:B:300:SER:HB3	2.21	0.40
1:B:216:HIS:CE1	1:B:366:PHE:HE1	2.39	0.40
1:B:259:LYS:HE2	1:B:259:LYS:N	2.35	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	422/481 (88%)	416 (99%)	5 (1%)	1 (0%)	47	37
1	B	407/481 (85%)	397 (98%)	10 (2%)	0	100	100
All	All	829/962 (86%)	813 (98%)	15 (2%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	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	341/385 (89%)	315 (92%)	26 (8%)	13	4
1	B	330/385 (86%)	295 (89%)	35 (11%)	6	2
All	All	671/770 (87%)	610 (91%)	61 (9%)	9	3

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	34	MET
1	A	37	LYS
1	A	45	SER
1	A	88	LYS
1	A	92	ILE
1	A	101	LEU
1	A	119	ARG
1	A	159	ARG
1	A	167	ASP
1	A	200	ILE
1	A	253	VAL
1	A	259	LYS
1	A	260	LEU
1	A	261	ARG
1	A	263	GLU
1	A	271	GLN
1	A	294	GLU
1	A	300	SER
1	A	310	LEU
1	A	311	THR
1	A	367	LYS
1	A	406	ARG
1	A	413	ARG
1	A	448	ARG
1	A	461	LEU
1	B	8	THR
1	B	12	ARG
1	B	18	ARG
1	B	34	MET
1	B	41	ARG
1	B	92	ILE
1	B	106	LEU
1	B	119	ARG
1	B	121	VAL

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Mol	Chain	Res	Type
1	B	159	ARG
1	B	217	SER
1	B	256	LEU
1	B	259	LYS
1	B	260	LEU
1	B	263	GLU
1	B	296	TRP
1	B	297	TYR
1	B	299	LYS
1	B	349	LYS
1	B	355	GLN
1	B	367	LYS
1	B	372	ARG
1	B	386	ILE
1	B	392	ILE
1	B	394	ASP
1	B	396	LEU
1	B	409	GLU
1	B	413	ARG
1	B	422	THR
1	B	425	GLU
1	B	439	SER
1	B	443	LYS
1	B	447	LEU
1	B	448	ARG
1	B	461	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	428	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	504	-	5,5,5	0.26	0	5,5,5	0.43	0
3	FAD	A	502	-	51,58,58	2.08	15 (29%)	60,89,89	2.61	18 (30%)
4	GOL	A	505	-	5,5,5	0.58	0	5,5,5	0.55	0
3	FAD	B	502	-	51,58,58	2.28	15 (29%)	60,89,89	2.46	14 (23%)
5	IMD	B	504	-	3,5,5	0.29	0	4,5,5	0.98	0
2	26J	A	501	1	28,33,33	1.98	5 (17%)	35,48,48	2.68	18 (51%)
4	GOL	B	503	-	5,5,5	0.28	0	5,5,5	0.96	0
4	GOL	A	503	-	5,5,5	0.39	0	5,5,5	0.96	0
2	26J	B	501	1	28,33,33	1.28	2 (7%)	35,48,48	2.66	16 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	504	-	-	0/4/4/4	-
3	FAD	A	502	-	-	3/30/50/50	0/6/6/6
4	GOL	A	505	-	-	0/4/4/4	-
3	FAD	B	502	-	-	0/30/50/50	0/6/6/6
5	IMD	B	504	-	-	-	0/1/1/1
2	26J	A	501	1	-	3/12/34/34	0/3/4/4
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
2	26J	B	501	1	-	1/12/34/34	0/3/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	FAD	C4X-C10	9.45	1.48	1.38
3	A	502	FAD	C10-N1	5.85	1.40	1.33
2	A	501	26J	OAD-CAZ	5.79	1.39	1.24
2	A	501	26J	CAY-NBF	5.43	1.40	1.32
3	A	502	FAD	C9-C8	4.60	1.49	1.37
2	B	501	26J	OAD-CAZ	4.31	1.35	1.24
3	A	502	FAD	O4'-C4'	4.22	1.52	1.43
3	B	502	FAD	C4X-N5	4.16	1.39	1.33
3	A	502	FAD	C4X-N5	3.95	1.39	1.33
2	A	501	26J	CAJ-CAX	3.93	1.43	1.38
3	B	502	FAD	C7M-C7	3.91	1.58	1.51
3	A	502	FAD	C4X-C10	3.91	1.42	1.38
3	A	502	FAD	O2B-C2B	3.90	1.52	1.43
3	B	502	FAD	O4B-C1B	3.81	1.46	1.41
3	B	502	FAD	C9A-C5X	3.66	1.49	1.42
3	A	502	FAD	C2A-N3A	3.56	1.37	1.32
3	B	502	FAD	C10-N1	3.55	1.37	1.33
3	A	502	FAD	C9A-C5X	3.43	1.49	1.42
3	A	502	FAD	O4B-C1B	3.40	1.45	1.41
3	B	502	FAD	C5A-C4A	3.21	1.49	1.40
2	B	501	26J	CAY-NBF	3.18	1.37	1.32
3	B	502	FAD	C8-C7	3.09	1.48	1.40
2	A	501	26J	CAL-NBF	2.88	1.51	1.46
3	A	502	FAD	C2-N1	-2.83	1.32	1.38
3	B	502	FAD	C4-N3	2.82	1.37	1.33
3	B	502	FAD	C2A-N1A	2.58	1.38	1.33
3	B	502	FAD	C2A-N3A	2.54	1.36	1.32
3	B	502	FAD	C2B-C1B	-2.53	1.49	1.53
3	B	502	FAD	C9A-N10	2.51	1.41	1.38
3	A	502	FAD	C8-C7	2.48	1.47	1.40
3	A	502	FAD	C6-C7	2.45	1.44	1.37
3	B	502	FAD	P-O2P	-2.37	1.44	1.55
3	B	502	FAD	C2-N1	-2.27	1.33	1.38
3	A	502	FAD	C9A-N10	2.26	1.41	1.38
3	A	502	FAD	O3B-C3B	2.17	1.48	1.43
2	A	501	26J	CAZ-NAR	2.08	1.36	1.33
3	A	502	FAD	C7M-C7	2.02	1.55	1.51

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	FAD	C4-C4X-C10	-7.97	114.67	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	FAD	C4X-N5-C5X	7.97	124.74	116.77
3	B	502	FAD	C4-N3-C2	7.11	121.14	115.14
3	A	502	FAD	C4-C4X-C10	-6.97	115.34	119.95
3	A	502	FAD	C4-N3-C2	6.61	120.72	115.14
3	B	502	FAD	C10-C4X-N5	6.59	125.81	121.26
3	A	502	FAD	C4-C4X-N5	6.52	126.05	118.60
3	B	502	FAD	C1'-N10-C9A	6.51	123.42	118.29
2	A	501	26J	CAN-NBH-CAO	6.46	123.37	108.83
2	A	501	26J	CAX-CAJ-CAW	-6.11	116.69	121.96
3	B	502	FAD	C5X-C9A-N10	6.11	122.14	117.72
3	A	502	FAD	C5X-C9A-N10	-5.35	113.84	117.72
2	B	501	26J	CAL-NBF-CAM	5.34	123.31	111.52
2	B	501	26J	CAL-CAN-NBH	-5.21	99.94	110.64
3	A	502	FAD	C10-C4X-N5	-5.09	117.73	121.26
3	A	502	FAD	O4'-C4'-C5'	-4.73	99.28	109.92
2	B	501	26J	CAN-NBH-C30	4.65	124.70	111.20
2	A	501	26J	CAZ-NAR-CAY	4.52	126.09	115.04
2	B	501	26J	CAO-CAM-NBF	-4.50	101.95	110.70
2	B	501	26J	CAM-CAO-NBH	-4.40	101.62	110.64
2	B	501	26J	CAZ-NAR-CAY	4.15	125.18	115.04
2	A	501	26J	CAZ-CBA-CBB	4.00	122.99	119.98
2	B	501	26J	CBA-CAZ-NAR	3.90	127.12	124.40
3	B	502	FAD	C9A-N10-C10	-3.84	116.89	121.91
3	A	502	FAD	N3A-C2A-N1A	-3.82	122.70	128.68
2	B	501	26J	CAN-NBH-CAO	3.77	117.31	108.83
3	B	502	FAD	O4'-C4'-C3'	3.77	118.26	109.10
3	A	502	FAD	O2'-C2'-C3'	-3.75	99.99	109.10
2	A	501	26J	CAO-CAM-NBF	-3.72	103.47	110.70
2	A	501	26J	C31-C30-NBH	-3.71	109.43	114.65
2	B	501	26J	NAR-CAY-NBF	3.55	122.57	116.80
2	A	501	26J	CAN-CAL-NBF	-3.53	103.84	110.70
3	B	502	FAD	N3A-C2A-N1A	-3.51	123.19	128.68
3	A	502	FAD	C5B-C4B-C3B	-3.48	102.14	115.18
2	B	501	26J	CBB-CAX-NBE	3.47	120.35	116.50
2	A	501	26J	FAG-CBG-CAW	-3.42	105.43	112.93
2	A	501	26J	NAR-CAY-NBF	3.19	121.98	116.80
2	B	501	26J	CAN-CAL-NBF	-3.00	104.88	110.70
3	A	502	FAD	C1'-C2'-C3'	-2.99	101.43	109.79
2	A	501	26J	CAK-CAW-CBG	-2.86	115.91	120.15
3	B	502	FAD	C1B-N9A-C4A	-2.83	121.67	126.64
3	A	502	FAD	O4B-C4B-C3B	2.76	110.58	105.11
2	A	501	26J	CAN-NBH-C30	2.71	119.06	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	26J	CAL-NBF-CAM	2.63	117.33	111.52
3	B	502	FAD	O3'-C3'-C2'	-2.60	102.52	108.81
3	B	502	FAD	C2A-N1A-C6A	2.60	123.19	118.75
3	A	502	FAD	O3B-C3B-C4B	-2.49	103.85	111.05
3	A	502	FAD	O4'-C4'-C3'	-2.47	103.11	109.10
3	A	502	FAD	N6A-C6A-N1A	2.37	123.50	118.57
2	A	501	26J	C34-C35-C36	2.36	116.22	111.42
3	B	502	FAD	C4X-C4-N3	-2.35	120.21	123.43
3	B	502	FAD	C4X-C10-N10	-2.33	117.91	120.30
2	A	501	26J	CBB-CAK-NBE	2.32	119.07	116.50
2	B	501	26J	CAW-CAK-CBA	-2.31	120.19	122.52
3	A	502	FAD	C4X-C4-N3	-2.25	120.36	123.43
3	A	502	FAD	C9A-N10-C10	2.24	124.84	121.91
2	A	501	26J	CAO-NBH-C30	2.19	117.55	111.20
2	A	501	26J	C33-C32-C31	2.18	116.28	112.15
2	B	501	26J	CAO-NBH-C30	2.16	117.46	111.20
2	B	501	26J	CAZ-CBA-CBB	2.14	121.59	119.98
3	A	502	FAD	C4X-C10-N10	-2.11	118.13	120.30
3	B	502	FAD	C8M-C8-C9	-2.08	115.38	120.34
2	B	501	26J	FAG-CBG-CAW	-2.06	108.40	112.93
2	B	501	26J	CAX-CAJ-CAW	-2.05	120.19	121.96
2	A	501	26J	CAK-CAW-CAJ	2.03	122.48	118.69
2	A	501	26J	CAW-CAK-CBA	-2.01	120.49	122.52

There are no chirality outliers.

All (11) torsion outliers are listed below:

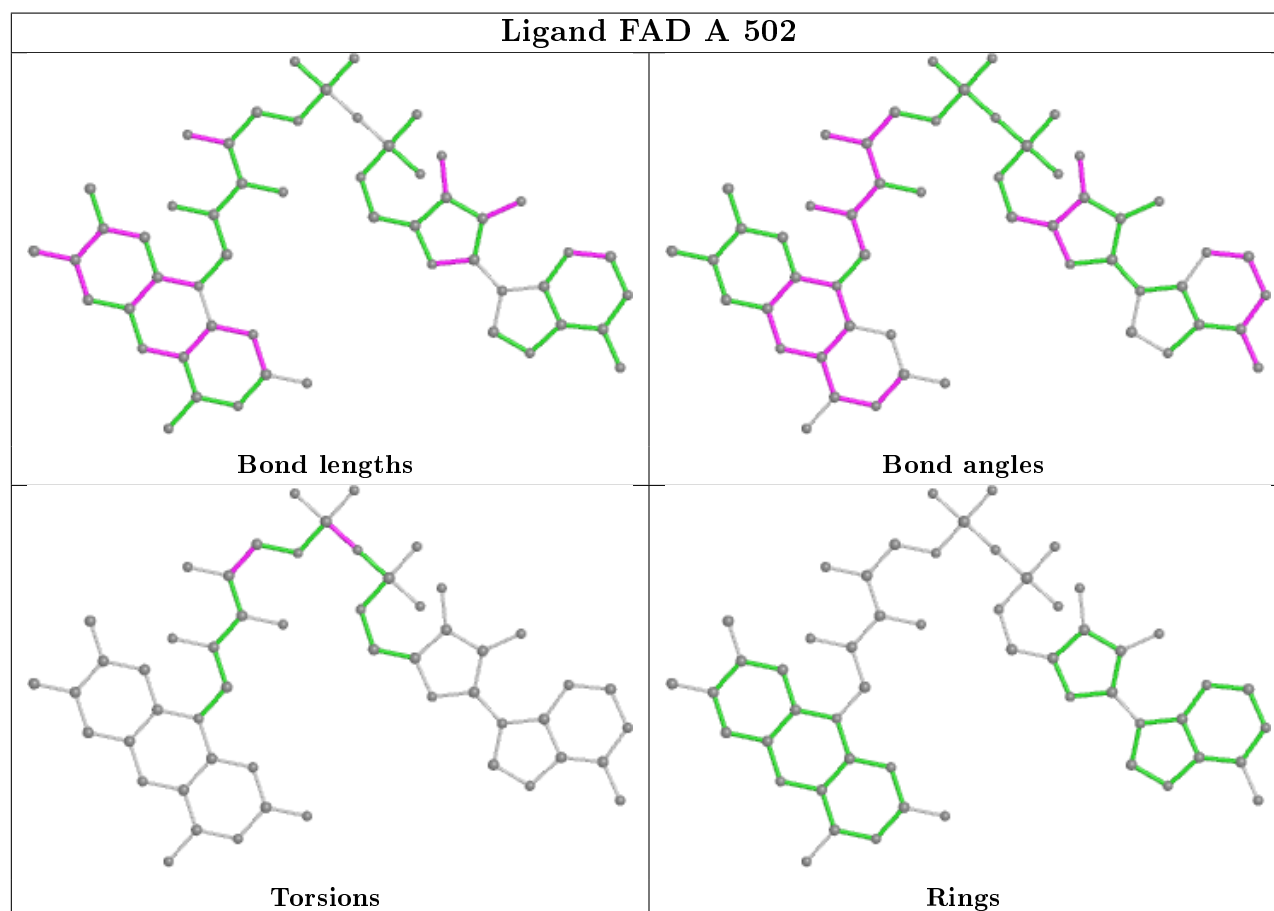
Mol	Chain	Res	Type	Atoms
4	B	503	GOL	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-C3
4	A	503	GOL	C1-C2-C3-O3
4	A	503	GOL	O2-C2-C3-O3
2	B	501	26J	C31-C30-NBH-CAO
2	A	501	26J	NBH-C30-C31-C36
2	A	501	26J	NBH-C30-C31-C32
3	A	502	FAD	PA-O3P-P-O1P
2	A	501	26J	C31-C30-NBH-CAO
3	A	502	FAD	PA-O3P-P-O2P
3	A	502	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

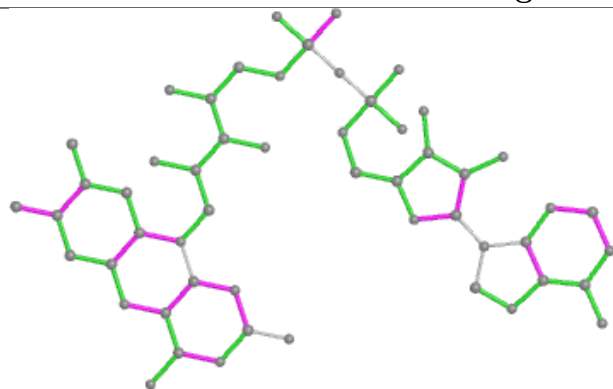
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	GOL	1	0
5	B	504	IMD	2	0
2	A	501	26J	3	0
4	B	503	GOL	3	0
4	A	503	GOL	1	0
2	B	501	26J	1	0

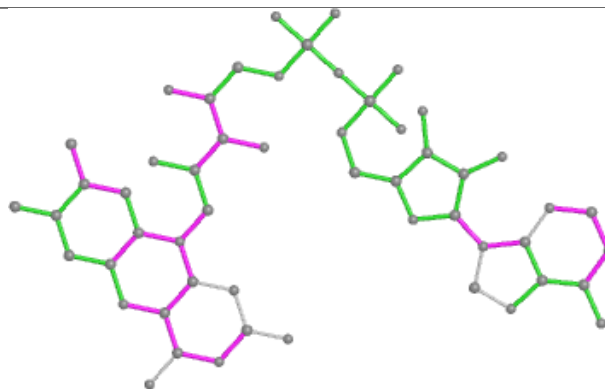
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



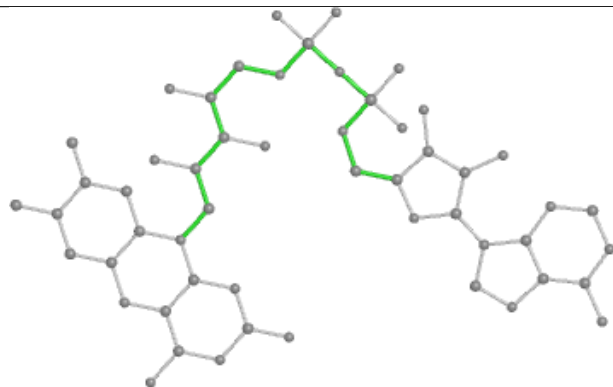
Ligand FAD B 502



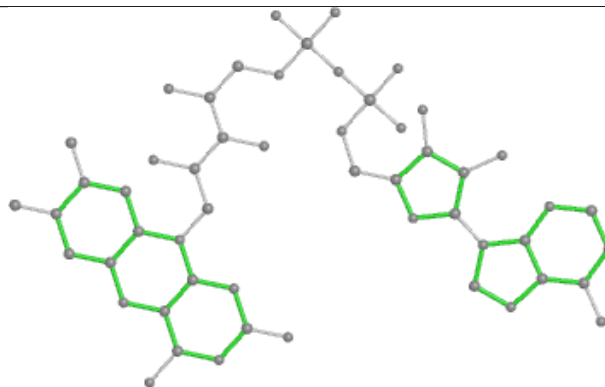
Bond lengths



Bond angles

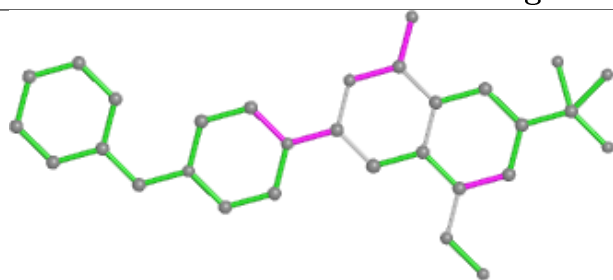


Torsions

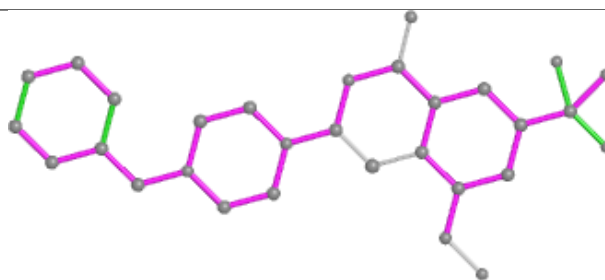


Rings

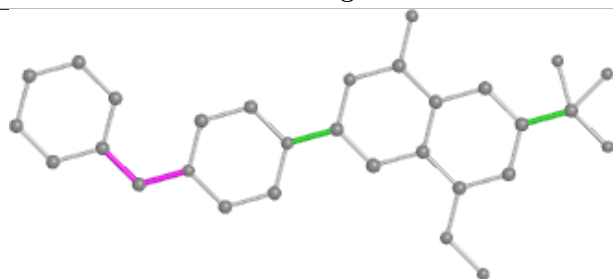
Ligand 26J A 501



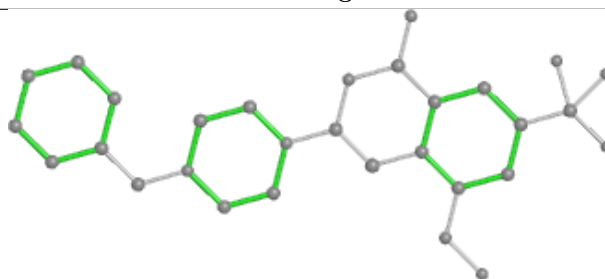
Bond lengths



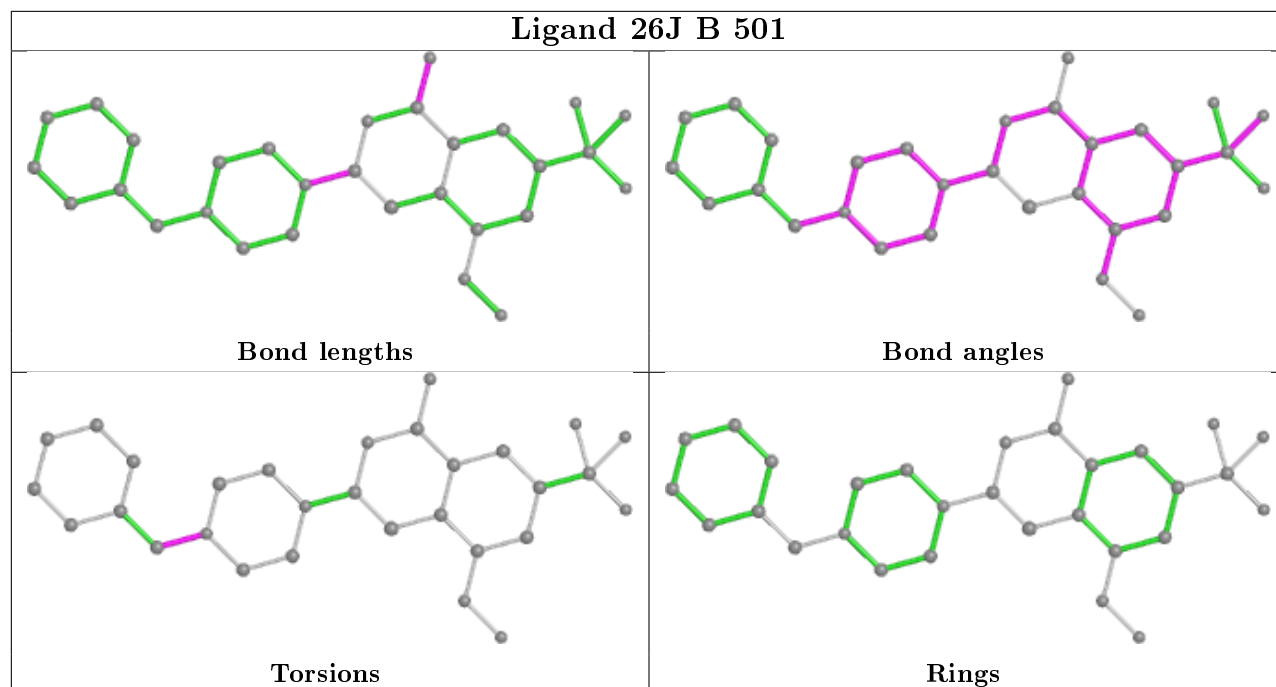
Bond angles



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	428/481 (88%)	-0.06	12 (2%) 53 54	19, 31, 63, 108	0
1	B	413/481 (85%)	-0.07	12 (2%) 51 53	21, 37, 69, 106	0
All	All	841/962 (87%)	-0.07	24 (2%) 51 53	19, 33, 66, 108	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	GLY	11.0
1	B	46	GLY	5.8
1	A	314	TYR	5.7
1	A	6	ALA	5.4
1	A	7	THR	5.0
1	A	47	GLY	4.3
1	B	297	TYR	4.3
1	B	270	PRO	3.6
1	A	267	PHE	3.1
1	B	362	PHE	3.1
1	B	37	LYS	3.1
1	B	269	ALA	3.1
1	B	10	ALA	2.9
1	A	270	PRO	2.7
1	B	9	THR	2.6
1	B	12	ARG	2.6
1	B	19	THR	2.4
1	A	18	ARG	2.4
1	A	311	THR	2.3
1	A	362	PHE	2.3
1	A	269	ALA	2.2
1	B	18	ARG	2.2
1	B	42	VAL	2.2
1	A	313	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

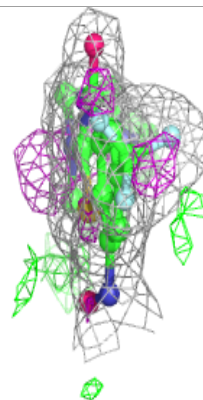
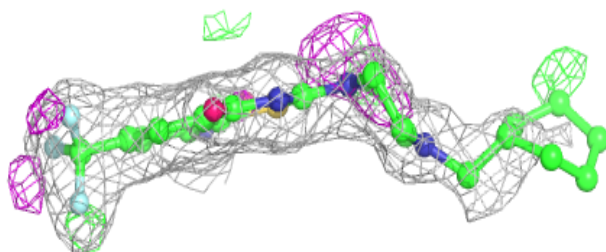
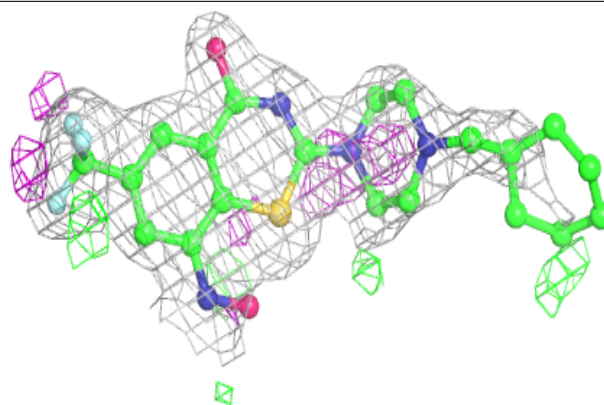
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	505	6/6	0.73	0.17	54,66,70,76	0
4	GOL	A	504	6/6	0.75	0.29	54,75,77,90	0
4	GOL	B	503	6/6	0.85	0.26	40,44,60,61	0
4	GOL	A	503	6/6	0.91	0.18	61,63,66,81	0
2	26J	A	501	30/30	0.95	0.15	32,38,88,92	0
5	IMD	B	504	5/5	0.96	0.12	44,45,46,53	0
2	26J	B	501	30/30	0.96	0.13	33,43,87,88	0
3	FAD	B	502	53/53	0.98	0.10	21,28,32,33	0
3	FAD	A	502	53/53	0.99	0.08	17,23,25,27	0

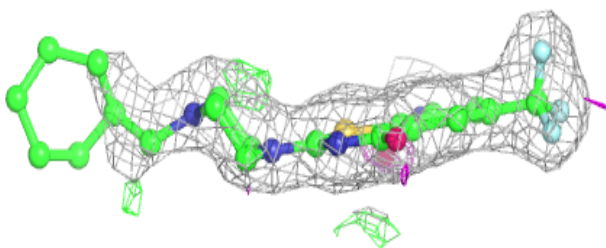
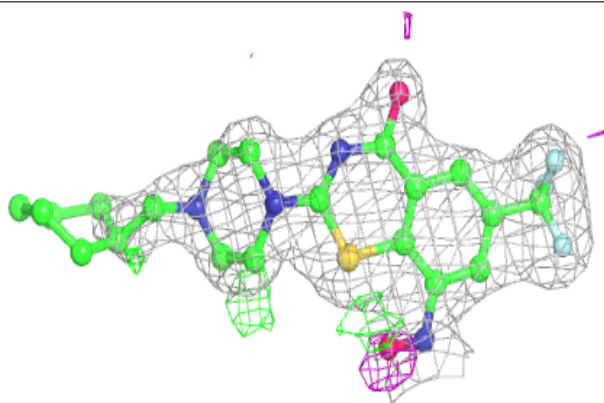
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 26J A 501:

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

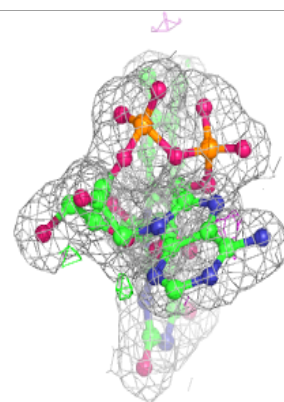
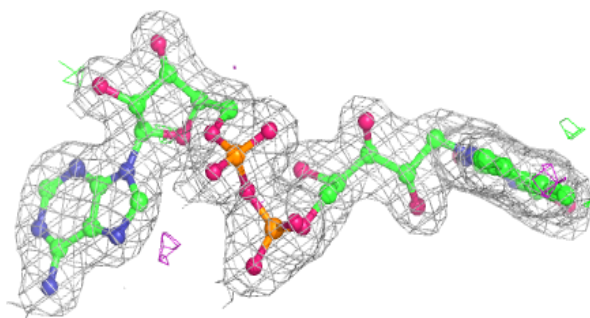
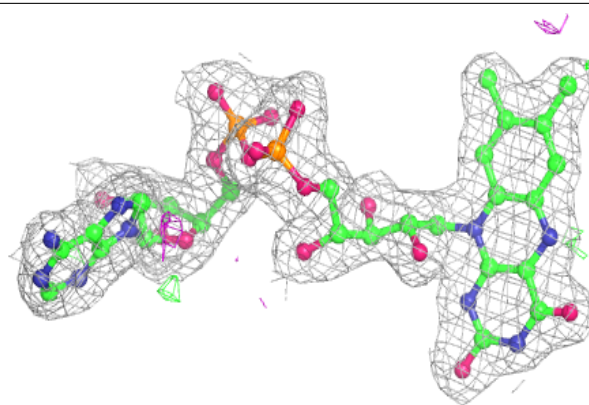
**Electron density around 26J B 501:**

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

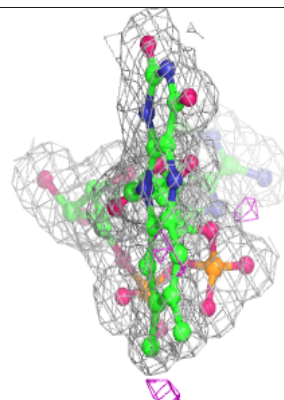
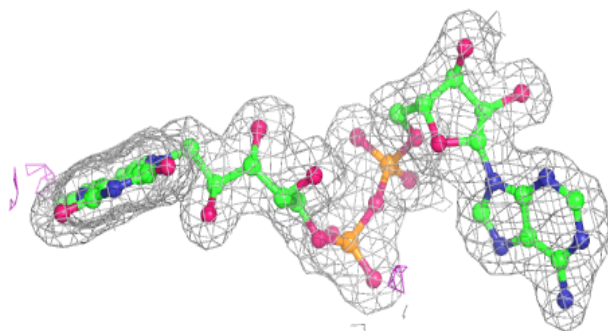
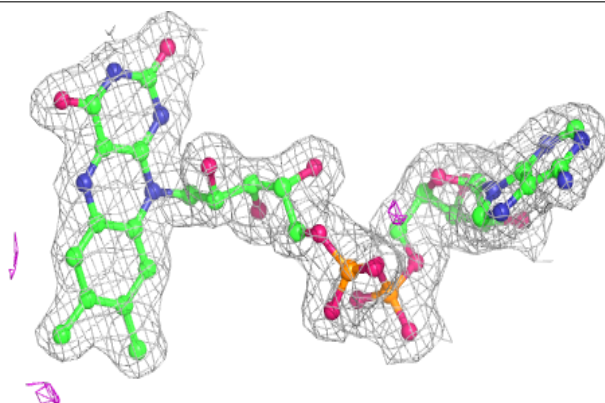


Electron density around FAD B 502:

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

**Electron density around FAD A 502:**

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



6.5 Other polymers

There are no such residues in this entry.