Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 09:24 AM EDT

PDB ID	:	5UAO
Title	:	Crystal structure of MibH, a lathipeptide tryptophan 5-halogenase
Authors	:	Cogan, D.P.; Nair, S.K.
Deposited on	:	2016-12-19
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 (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:

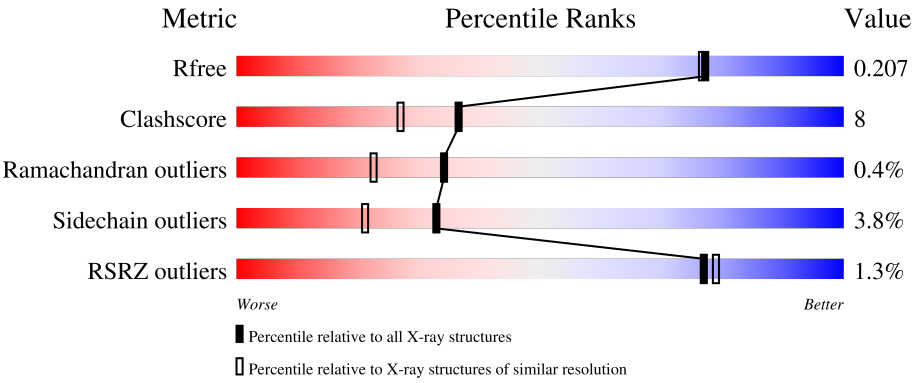
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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 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	541	86% 9%
1	B	541	81% 11% 5%
1	C	541	78% 15% 5%
1	D	541	79% 14% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	D	602	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17363 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.

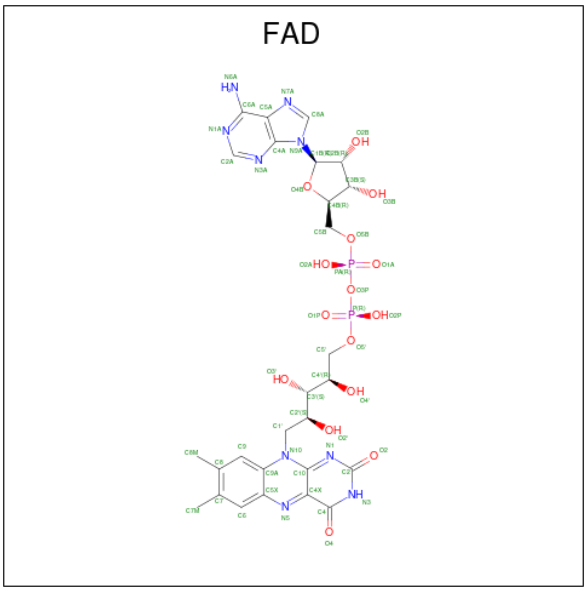
- Molecule 1 is a protein called Tryptophane-5-halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4003	2543	714	733	13			
1	B	516	Total	C	N	O	S	0	0	0
			3977	2528	711	725	13			
1	C	514	Total	C	N	O	S	0	0	0
			3967	2523	709	722	13			
1	D	514	Total	C	N	O	S	0	0	0
			3961	2520	706	722	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP W2EQU4
B	1	MET	-	initiating methionine	UNP W2EQU4
C	1	MET	-	initiating methionine	UNP W2EQU4
D	1	MET	-	initiating methionine	UNP W2EQU4

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

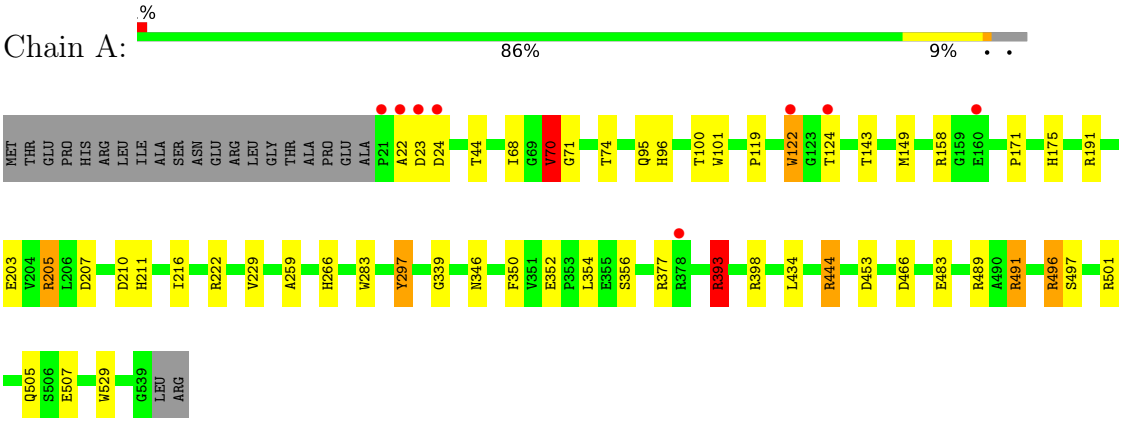
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	349	Total	O	0	0
			349	349		
4	B	353	Total	O	0	0
			353	353		
4	C	284	Total	O	0	0
			284	284		
4	D	361	Total	O	0	0
			361	361		

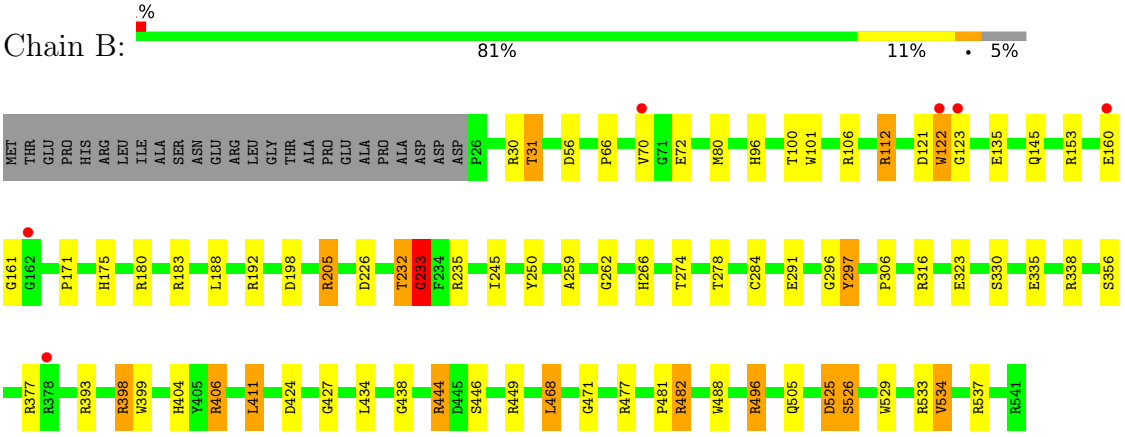
3 Residue-property plots (i)

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.

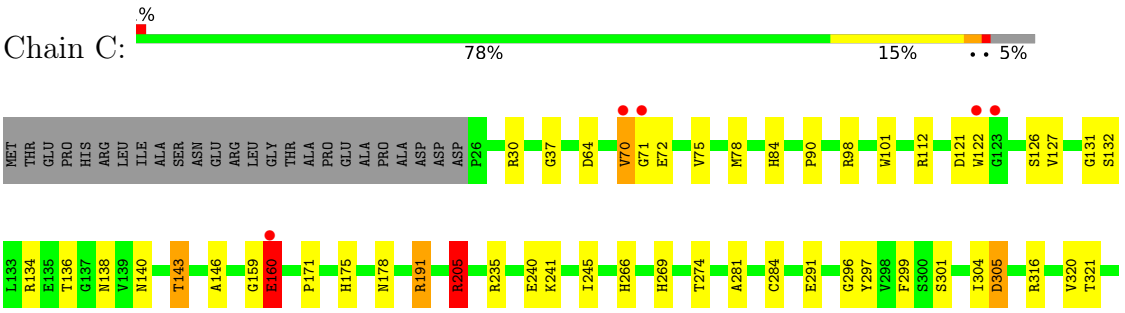
• Molecule 1: Tryptophane-5-halogenase

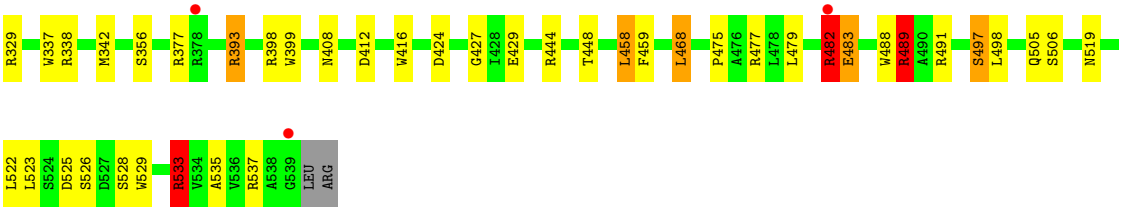


• Molecule 1: Tryptophane-5-halogenase



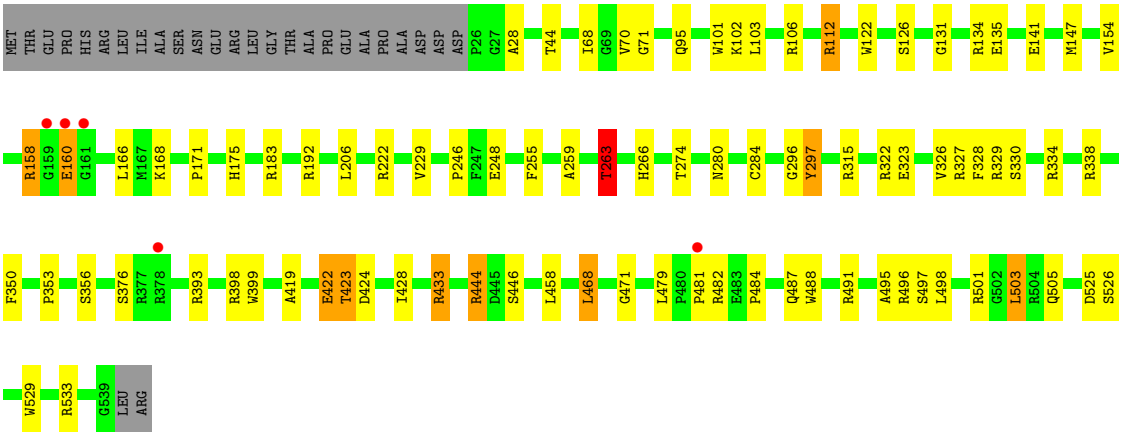
• Molecule 1: Tryptophane-5-halogenase





• Molecule 1: Tryptophane-5-halogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.44Å 87.89Å 100.63Å 64.58° 69.90° 76.26°	Depositor
Resolution (Å)	87.38 – 1.88 74.33 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.8 (87.38-1.88) 97.8 (74.33-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.156 , 0.204 0.162 , 0.207	Depositor DCC
R_{free} test set	8240 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.9	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	0.97	EDS
Total number of atoms	17363	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.92	1/4109 (0.0%)	1.05	13/5599 (0.2%)
1	B	0.96	1/4081 (0.0%)	1.03	22/5559 (0.4%)
1	C	0.90	1/4072 (0.0%)	1.00	17/5547 (0.3%)
1	D	0.95	1/4066 (0.0%)	1.12	22/5540 (0.4%)
All	All	0.93	4/16328 (0.0%)	1.05	74/22245 (0.3%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	TRP	CB-CG	-8.31	1.35	1.50
1	D	393	ARG	CD-NE	-7.12	1.34	1.46
1	C	301	SER	CB-OG	-6.77	1.33	1.42
1	B	233	GLY	N-CA	-5.80	1.37	1.46

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	ALA	N-CA-CB	-25.74	74.07	110.10
1	D	393	ARG	NE-CZ-NH2	-23.93	108.33	120.30
1	D	393	ARG	NE-CZ-NH1	15.01	127.81	120.30
1	A	22	ALA	N-CA-C	13.53	147.52	111.00
1	C	393	ARG	NE-CZ-NH2	-11.73	114.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	496	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	A	444	ARG	NE-CZ-NH1	-10.80	114.90	120.30
1	D	423	THR	N-CA-CB	9.90	129.11	110.30
1	C	393	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	C	468	LEU	CA-CB-CG	-9.07	94.44	115.30
1	A	393	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	D	468	LEU	CA-CB-CG	-8.55	95.64	115.30
1	D	192	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	D	112	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	D	134	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	C	489	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	D	393	ARG	CG-CD-NE	-7.93	95.14	111.80
1	D	112	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	B	496	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	B	406	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	B	406	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	316	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	C	424	ASP	CB-CG-OD1	7.36	124.93	118.30
1	D	134	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	D	192	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	C	525	ASP	CB-CG-OD1	-7.24	111.79	118.30
1	B	232	THR	CA-C-N	6.94	130.07	116.20
1	B	316	ARG	CG-CD-NE	-6.68	97.77	111.80
1	A	444	ARG	NE-CZ-NH2	6.63	123.62	120.30
1	A	466	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	444	ARG	CG-CD-NE	-6.56	98.02	111.80
1	C	205	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	424	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	D	393	ARG	CD-NE-CZ	6.43	132.61	123.60
1	D	263	THR	N-CA-CB	-6.36	98.22	110.30
1	A	393	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	232	THR	O-C-N	-6.33	112.44	123.20
1	D	424	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	305	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	422	GLU	N-CA-C	-6.07	94.62	111.00
1	B	122	TRP	CA-CB-CG	-6.04	102.21	113.70
1	B	232	THR	C-N-CA	6.01	134.92	122.30
1	C	424	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	78	MET	CG-SD-CE	-5.98	90.63	100.20
1	A	70	VAL	N-CA-C	5.94	127.05	111.00
1	A	496	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	424	ASP	CB-CG-OD1	5.89	123.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	327	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	56	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	30	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	433	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	232	THR	N-CA-C	5.74	126.50	111.00
1	C	191	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	468	LEU	CA-CB-CG	-5.62	102.36	115.30
1	C	329	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	D	423	THR	N-CA-C	-5.59	95.90	111.00
1	B	112	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	B	434	LEU	CA-CB-CG	5.58	128.14	115.30
1	B	106	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	37	GLY	C-N-CA	-5.52	110.71	122.30
1	D	106	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	112	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	C	316	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	191	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	491	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	153	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	489	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	23	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	255	PHE	CB-CA-C	-5.20	100.01	110.40
1	C	533	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	235	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	180	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	103	LEU	CB-CG-CD2	5.04	119.56	111.00
1	D	315	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	232	THR	Peptide

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	4003	0	3916	50	0
1	B	3977	0	3902	74	0
1	C	3967	0	3892	63	1
1	D	3961	0	3881	57	1
2	A	53	0	31	14	0
2	D	53	0	31	2	0
3	A	1	0	0	1	0
3	D	1	0	0	2	0
4	A	349	0	0	29	0
4	B	353	0	0	31	0
4	C	284	0	0	24	0
4	D	361	0	0	23	0
All	All	17363	0	15653	250	1

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 8.

All (250) 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:D:280:ASN:HB3	4:D:955:HOH:O	1.39	1.20
1:D:95:GLN:HG2	4:D:896:HOH:O	1.55	1.06
1:C:281:ALA:HB3	1:C:304:ILE:HD13	1.37	1.03
1:C:98:ARG:NH2	1:C:291:GLU:OE2	1.93	1.02
1:B:66:PRO:O	4:B:601:HOH:O	1.79	1.00
1:B:496:ARG:HG3	4:B:603:HOH:O	1.65	0.96
1:B:477:ARG:CB	4:B:925:HOH:O	2.16	0.94
1:D:166:LEU:HG	4:D:1030:HOH:O	1.66	0.93
1:B:122:TRP:CZ3	4:B:888:HOH:O	2.22	0.93
1:A:393:ARG:NH2	4:A:703:HOH:O	2.04	0.88
1:D:526:SER:O	1:D:533:ARG:NH1	2.09	0.86
1:A:71:GLY:N	4:A:701:HOH:O	1.78	0.85
1:B:245:ILE:HD11	1:B:338:ARG:HD2	1.58	0.85
1:B:404:HIS:CD2	1:B:468:LEU:HD21	2.13	0.84
1:A:497:SER:OG	1:A:501:ARG:NH1	2.10	0.83
1:D:323:GLU:CB	4:D:804:HOH:O	2.26	0.83
1:A:101:TRP:H	1:A:505:GLN:HE22	1.24	0.82
2:A:601:FAD:H3'	4:A:960:HOH:O	1.78	0.82
1:A:207:ASP:OD1	1:A:211:HIS:HD2	1.62	0.81
1:B:496:ARG:NE	4:B:603:HOH:O	2.12	0.80
1:A:352:GLU:OE2	4:A:702:HOH:O	1.99	0.80
1:B:121:ASP:HB2	4:B:624:HOH:O	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:THR:HG22	1:C:146:ALA:H	1.50	0.77
1:D:101:TRP:H	1:D:505:GLN:HE22	1.33	0.77
1:B:356:SER:OG	4:B:602:HOH:O	2.01	0.77
1:A:74:THR:HB	4:A:905:HOH:O	1.83	0.77
1:C:281:ALA:CB	1:C:304:ILE:HD13	2.15	0.77
1:A:124:THR:HB	4:A:920:HOH:O	1.83	0.76
1:A:496:ARG:NH2	4:A:705:HOH:O	2.17	0.76
1:C:393:ARG:NH2	4:C:601:HOH:O	2.01	0.76
1:A:71:GLY:C	4:A:711:HOH:O	2.24	0.75
1:C:178:ASN:ND2	4:C:603:HOH:O	2.19	0.74
1:D:444:ARG:NH1	4:D:703:HOH:O	2.20	0.74
2:A:601:FAD:C3'	4:A:960:HOH:O	2.34	0.73
1:B:31:THR:HG21	4:B:834:HOH:O	1.88	0.73
1:B:101:TRP:H	1:B:505:GLN:HE22	1.37	0.73
1:B:262:GLY:HA2	1:B:323:GLU:HG3	1.70	0.72
1:C:205:ARG:HD3	4:C:728:HOH:O	1.89	0.72
1:B:335:GLU:OE1	1:B:338:ARG:NH1	2.23	0.71
1:C:112:ARG:NH1	1:C:138:ASN:OD1	2.25	0.69
1:D:484:PRO:O	4:D:701:HOH:O	2.11	0.68
1:B:496:ARG:HD3	4:B:719:HOH:O	1.92	0.68
1:A:356:SER:HA	3:A:602:CL:CL	2.31	0.67
1:D:166:LEU:CG	4:D:1030:HOH:O	2.33	0.67
1:B:444:ARG:HG2	1:B:444:ARG:HH11	1.60	0.67
1:C:483:GLU:OE2	1:C:491:ARG:NH2	2.28	0.66
1:D:330:SER:OG	4:D:702:HOH:O	2.13	0.66
1:D:122:TRP:O	1:D:126:SER:OG	2.13	0.65
1:C:121:ASP:OD1	1:C:143:THR:HG21	1.95	0.65
1:C:235:ARG:O	4:C:602:HOH:O	2.13	0.65
1:A:350:PHE:HE1	2:A:601:FAD:C9	2.10	0.64
1:B:101:TRP:H	1:B:505:GLN:NE2	1.95	0.64
1:C:101:TRP:H	1:C:505:GLN:HE22	1.45	0.64
1:C:70:VAL:O	1:C:72:GLU:HG3	1.99	0.63
1:A:122:TRP:NE1	4:A:706:HOH:O	2.30	0.63
1:A:143:THR:HG23	4:A:924:HOH:O	1.99	0.63
1:D:322:ARG:NH2	4:D:709:HOH:O	2.30	0.63
1:B:404:HIS:CE1	1:B:468:LEU:HD22	2.34	0.63
1:B:198:ASP:HB3	4:B:729:HOH:O	1.99	0.63
1:C:444:ARG:HD3	1:C:479:LEU:HD11	1.81	0.63
1:B:393:ARG:NH1	4:B:606:HOH:O	2.27	0.62
1:B:205:ARG:HH11	1:B:205:ARG:HB2	1.65	0.62
4:A:978:HOH:O	1:C:477:ARG:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:NH2	1:B:306:PRO:HD3	2.15	0.61
1:A:434:LEU:HD13	4:A:992:HOH:O	2.00	0.61
1:C:477:ARG:N	4:C:606:HOH:O	2.34	0.61
1:B:70:VAL:O	1:B:72:GLU:HG3	2.00	0.61
1:B:183:ARG:NH2	4:B:609:HOH:O	2.32	0.61
1:D:329:ARG:N	4:D:708:HOH:O	2.30	0.61
1:A:70:VAL:O	4:A:704:HOH:O	2.16	0.60
1:C:90:PRO:HG3	1:C:523:LEU:HD11	1.81	0.60
1:C:305:ASP:HB2	4:C:821:HOH:O	2.01	0.60
1:A:207:ASP:OD1	1:A:211:HIS:CD2	2.50	0.60
1:B:330:SER:OG	4:B:604:HOH:O	2.16	0.60
1:D:444:ARG:CG	1:D:444:ARG:HH11	2.13	0.60
1:B:198:ASP:CB	4:B:729:HOH:O	2.50	0.59
1:B:226:ASP:OD1	1:B:377:ARG:NH2	2.35	0.59
1:C:121:ASP:OD1	1:C:143:THR:CG2	2.50	0.59
1:D:183:ARG:HD2	4:D:1019:HOH:O	2.03	0.59
1:B:121:ASP:O	1:B:122:TRP:CD1	2.56	0.59
1:D:350:PHE:HE1	2:D:601:FAD:C9	2.16	0.59
2:A:601:FAD:C2'	4:A:960:HOH:O	2.49	0.58
1:B:122:TRP:HZ2	4:B:778:HOH:O	1.85	0.58
1:A:205:ARG:CD	4:A:746:HOH:O	2.49	0.58
1:A:203:GLU:OE2	1:A:205:ARG:NH1	2.32	0.58
1:C:205:ARG:HG3	1:C:205:ARG:HH11	1.67	0.58
1:D:444:ARG:HH11	1:D:444:ARG:HG3	1.69	0.58
1:D:122:TRP:CD1	4:D:813:HOH:O	2.52	0.58
2:A:601:FAD:O4'	2:A:601:FAD:O2'	2.13	0.57
1:D:166:LEU:CD1	4:D:1030:HOH:O	2.52	0.57
1:C:134:ARG:NH2	1:C:479:LEU:O	2.38	0.57
1:A:346:ASN:ND2	2:A:601:FAD:H5'1	2.20	0.57
1:A:434:LEU:O	1:A:444:ARG:NH1	2.38	0.57
1:B:404:HIS:CD2	1:B:468:LEU:CD2	2.87	0.57
1:B:444:ARG:HG2	1:B:444:ARG:NH1	2.19	0.57
1:A:434:LEU:HB3	4:A:992:HOH:O	2.05	0.56
1:B:526:SER:O	1:B:533:ARG:NH2	2.32	0.56
1:B:496:ARG:CD	4:B:719:HOH:O	2.50	0.56
1:D:28:ALA:HA	1:D:376:SER:HB3	1.87	0.56
1:C:412:ASP:HB3	4:C:798:HOH:O	2.05	0.55
1:C:429:GLU:HB3	4:C:641:HOH:O	2.06	0.55
1:A:191:ARG:HD3	4:A:967:HOH:O	2.07	0.55
1:B:31:THR:CG2	1:B:226:ASP:H	2.19	0.55
1:A:101:TRP:H	1:A:505:GLN:NE2	2.00	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:HG3	4:B:753:HOH:O	2.07	0.55
1:A:96:HIS:HD2	4:A:1007:HOH:O	1.89	0.55
1:A:68:ILE:HG21	2:A:601:FAD:H4'	1.89	0.55
1:A:483:GLU:OE2	1:A:491:ARG:NH2	2.37	0.55
1:C:482:ARG:CZ	1:C:482:ARG:HB2	2.37	0.54
1:D:71:GLY:HA2	2:D:601:FAD:C4X	2.37	0.54
1:D:175:HIS:HE1	1:D:274:THR:OG1	1.91	0.54
1:C:90:PRO:HB2	1:C:519:ASN:HB3	1.89	0.54
1:D:356:SER:HA	3:D:602:CL:CL	2.45	0.54
1:C:537:ARG:HD2	4:C:859:HOH:O	2.07	0.54
1:D:68:ILE:HD11	1:D:326:VAL:HG13	1.89	0.54
1:B:444:ARG:HH11	1:B:444:ARG:CG	2.21	0.53
1:D:248:GLU:HG3	4:D:704:HOH:O	2.08	0.53
1:D:122:TRP:HZ3	4:D:771:HOH:O	1.89	0.53
1:D:328:PHE:CD1	1:D:350:PHE:HE2	2.25	0.53
1:C:205:ARG:HH11	1:C:205:ARG:CG	2.20	0.53
1:A:350:PHE:HE1	2:A:601:FAD:H9	1.72	0.53
1:C:101:TRP:H	1:C:505:GLN:NE2	2.05	0.53
1:B:529:TRP:O	1:B:534:VAL:HG21	2.09	0.53
1:A:377:ARG:HB2	4:A:977:HOH:O	2.10	0.52
1:B:171:PRO:HA	1:B:529:TRP:CE2	2.44	0.52
1:D:353:PRO:HA	3:D:602:CL:CL	2.46	0.52
1:D:246:PRO:C	4:D:704:HOH:O	2.48	0.52
1:D:433:ARG:HH11	1:D:433:ARG:HG3	1.75	0.52
1:C:458:LEU:HD23	4:C:830:HOH:O	2.08	0.52
1:D:131:GLY:HA3	1:D:488:TRP:CD1	2.45	0.51
1:D:141:GLU:OE2	1:D:496:ARG:NH1	2.43	0.51
1:A:205:ARG:HD3	4:A:746:HOH:O	2.10	0.51
2:A:601:FAD:C1'	4:A:960:HOH:O	2.58	0.51
1:C:75:VAL:HB	1:C:459:PHE:CZ	2.46	0.51
1:C:444:ARG:NH1	1:C:448:THR:HG21	2.25	0.51
1:D:158:ARG:HD2	1:D:503:LEU:HD11	1.93	0.51
1:D:433:ARG:NH1	4:D:716:HOH:O	2.44	0.51
1:B:112:ARG:NH1	1:B:471:GLY:HA2	2.26	0.51
1:B:31:THR:HG22	1:B:226:ASP:H	1.74	0.51
1:B:399:TRP:CE2	1:B:427:GLY:HA3	2.46	0.51
1:C:299:PHE:HB2	1:C:304:ILE:HD11	1.92	0.51
1:B:112:ARG:HH12	1:B:471:GLY:HA2	1.75	0.51
1:C:240:GLU:HB3	4:C:602:HOH:O	2.11	0.51
1:D:481:PRO:O	1:D:482:ARG:HB3	2.11	0.51
1:A:222:ARG:HD3	4:A:1014:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ILE:HD12	4:D:821:HOH:O	2.12	0.50
1:B:496:ARG:CG	4:B:603:HOH:O	2.37	0.50
1:C:64:ASP:C	4:C:646:HOH:O	2.49	0.50
1:D:147:MET:HE3	1:D:495:ALA:HB1	1.93	0.50
1:C:241:LYS:NZ	4:C:602:HOH:O	2.45	0.49
1:D:444:ARG:NH1	1:D:444:ARG:CG	2.70	0.49
1:C:245:ILE:HD11	1:C:338:ARG:HD2	1.94	0.49
1:C:304:ILE:HG21	4:C:836:HOH:O	2.12	0.49
1:C:537:ARG:CD	4:C:859:HOH:O	2.60	0.49
1:B:183:ARG:HD3	4:B:895:HOH:O	2.13	0.48
1:C:506:SER:HB3	4:C:638:HOH:O	2.13	0.48
1:C:171:PRO:HA	1:C:529:TRP:CE2	2.48	0.48
1:C:269:HIS:HD2	4:C:864:HOH:O	1.96	0.48
1:D:102:LYS:NZ	1:D:356:SER:OG	2.47	0.48
1:C:90:PRO:HG3	1:C:523:LEU:CD1	2.43	0.48
1:B:444:ARG:O	1:B:449:ARG:NH1	2.48	0.47
1:D:328:PHE:CD1	1:D:350:PHE:CE2	3.02	0.47
1:D:171:PRO:HA	1:D:529:TRP:CE2	2.50	0.47
1:B:80:MET:HE1	1:B:534:VAL:HG23	1.96	0.47
1:A:68:ILE:CG2	2:A:601:FAD:H4'	2.44	0.47
1:C:175:HIS:HE1	1:C:274:THR:OG1	1.98	0.47
1:A:259:ALA:HA	1:A:297:TYR:O	2.14	0.46
1:D:135:GLU:HG3	1:D:488:TRP:CZ3	2.50	0.46
1:D:168:LYS:NZ	1:D:525:ASP:OD2	2.44	0.46
1:C:131:GLY:HA3	1:C:488:TRP:CD1	2.51	0.46
1:C:489:ARG:HH11	1:C:489:ARG:CB	2.29	0.46
1:A:95:GLN:HG2	4:A:974:HOH:O	2.15	0.46
1:A:119:PRO:HB3	1:A:149:MET:CE	2.46	0.46
1:B:233:GLY:HA2	4:B:815:HOH:O	2.15	0.46
1:C:533:ARG:HB2	1:C:533:ARG:HH11	1.80	0.45
2:A:601:FAD:HO4'	2:A:601:FAD:H1'1	1.80	0.45
1:B:188:LEU:O	1:B:192:ARG:HG3	2.16	0.45
1:A:171:PRO:HA	1:A:529:TRP:CE2	2.50	0.45
1:B:96:HIS:HD2	4:B:878:HOH:O	1.99	0.45
1:B:534:VAL:HG13	4:B:821:HOH:O	2.16	0.45
1:C:497:SER:HB3	4:C:683:HOH:O	2.17	0.45
1:B:284:CYS:HA	1:B:296:GLY:O	2.16	0.45
1:A:211:HIS:HE1	4:A:971:HOH:O	1.99	0.45
1:C:140:ASN:HB2	4:C:689:HOH:O	2.17	0.45
1:B:161:GLY:C	4:B:625:HOH:O	2.55	0.45
1:C:64:ASP:HB2	4:C:634:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:SER:O	1:C:136:THR:HB	2.17	0.45
1:B:404:HIS:CG	1:B:468:LEU:CD2	2.99	0.45
1:B:404:HIS:CE1	1:B:468:LEU:CD2	3.00	0.44
1:C:337:TRP:HB2	1:C:342:MET:HG3	1.98	0.44
1:B:404:HIS:NE2	1:B:468:LEU:HD21	2.32	0.44
1:C:408:ASN:HB3	1:C:416:TRP:CZ3	2.50	0.44
1:D:419:ALA:O	1:D:422:GLU:O	2.36	0.44
1:C:399:TRP:CE2	1:C:427:GLY:HA3	2.52	0.44
1:C:444:ARG:NH1	4:C:619:HOH:O	2.50	0.44
1:A:158:ARG:NH1	1:A:507:GLU:OE2	2.51	0.44
1:B:160:GLU:OE1	1:B:160:GLU:HA	2.17	0.44
1:B:135:GLU:HG3	1:B:488:TRP:CZ3	2.53	0.44
1:B:121:ASP:CG	1:B:145:GLN:HB2	2.37	0.44
1:B:175:HIS:HE1	1:B:274:THR:OG1	2.00	0.44
1:B:393:ARG:NH1	4:B:610:HOH:O	2.34	0.44
1:C:84:HIS:CD2	1:C:535:ALA:HB2	2.53	0.44
1:C:284:CYS:HA	1:C:296:GLY:O	2.18	0.44
1:C:320:VAL:HG22	1:C:321:THR:O	2.18	0.44
1:D:122:TRP:HD1	4:D:813:HOH:O	1.95	0.44
1:A:283:TRP:CE2	1:A:354:LEU:HD13	2.53	0.43
1:D:44:THR:HG21	1:D:229:VAL:HG11	2.00	0.43
1:A:497:SER:HA	4:A:972:HOH:O	2.18	0.43
1:B:80:MET:CE	1:B:534:VAL:HG23	2.47	0.43
1:A:100:THR:OG1	1:A:175:HIS:HB2	2.18	0.43
1:C:475:PRO:O	4:C:604:HOH:O	2.21	0.43
1:D:329:ARG:HG2	4:D:708:HOH:O	2.18	0.43
1:D:497:SER:HB2	1:D:501:ARG:NH1	2.33	0.43
1:B:30:ARG:NE	4:B:611:HOH:O	2.35	0.43
1:C:159:GLY:O	1:C:160:GLU:C	2.56	0.43
1:B:259:ALA:HA	1:B:297:TYR:O	2.19	0.43
1:B:122:TRP:N	4:B:624:HOH:O	2.52	0.42
1:D:122:TRP:CZ3	4:D:771:HOH:O	2.55	0.42
1:B:278:THR:HG22	1:B:411:LEU:HD22	2.01	0.42
1:C:136:THR:HG21	4:C:689:HOH:O	2.18	0.42
1:B:250:TYR:CG	1:B:398:ARG:HG3	2.55	0.42
2:A:601:FAD:C2	4:A:711:HOH:O	2.68	0.42
1:C:522:LEU:O	1:C:528:SER:OG	2.32	0.42
1:D:284:CYS:HA	1:D:296:GLY:O	2.20	0.42
1:D:334:ARG:NE	4:D:728:HOH:O	2.53	0.42
1:D:263:THR:HG23	4:D:1000:HOH:O	2.19	0.42
1:A:210:ASP:O	1:A:339:GLY:HA3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ARG:NH1	1:D:471:GLY:O	2.52	0.41
1:D:160:GLU:N	1:D:160:GLU:OE1	2.53	0.41
1:B:477:ARG:CB	4:B:928:HOH:O	2.68	0.41
1:D:399:TRP:HB3	1:D:428:ILE:HB	2.03	0.41
1:B:122:TRP:CZ3	4:B:690:HOH:O	2.57	0.41
1:B:481:PRO:O	1:B:482:ARG:HB2	2.20	0.41
1:B:100:THR:OG1	1:B:175:HIS:HB2	2.20	0.41
1:A:119:PRO:HG3	4:A:924:HOH:O	2.20	0.41
1:A:122:TRP:CE2	4:A:706:HOH:O	2.70	0.41
1:B:31:THR:O	1:B:226:ASP:HB2	2.20	0.41
1:B:291:GLU:OE1	4:B:605:HOH:O	2.21	0.41
1:B:121:ASP:CB	4:B:624:HOH:O	2.55	0.40
1:A:44:THR:HG21	1:A:229:VAL:HG11	2.03	0.40
1:A:346:ASN:CG	2:A:601:FAD:H5'1	2.41	0.40
1:A:350:PHE:CE1	2:A:601:FAD:C9	2.97	0.40
1:A:497:SER:O	1:A:501:ARG:HG3	2.21	0.40
1:B:205:ARG:HH11	1:B:205:ARG:CB	2.33	0.40
1:D:101:TRP:H	1:D:505:GLN:NE2	2.09	0.40
1:A:216:ILE:HD12	1:A:222:ARG:HG2	2.03	0.40
1:B:205:ARG:HD3	4:B:867:HOH:O	2.22	0.40
1:C:127:VAL:O	1:C:491:ARG:NH1	2.54	0.40
1:C:377:ARG:HG3	4:C:647:HOH:O	2.21	0.40
1:D:259:ALA:HA	1:D:297:TYR:O	2.21	0.40

All (1) 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)
1:C:412:ASP:OD2	1:D:280:ASN:OD1[1_455]	2.02	0.18

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	517/541 (96%)	503 (97%)	14 (3%)	0	100	100
1	B	514/541 (95%)	497 (97%)	13 (2%)	4 (1%)	19	9
1	C	512/541 (95%)	486 (95%)	22 (4%)	4 (1%)	19	9
1	D	512/541 (95%)	500 (98%)	11 (2%)	1 (0%)	47	37
All	All	2055/2164 (95%)	1986 (97%)	60 (3%)	9 (0%)	34	22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	483	GLU
1	D	423	THR
1	B	233	GLY
1	C	71	GLY
1	C	160	GLU
1	B	525	ASP
1	C	482	ARG
1	B	123	GLY
1	B	438	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	404/423 (96%)	396 (98%)	8 (2%)	55	47
1	B	401/423 (95%)	387 (96%)	14 (4%)	36	24
1	C	400/423 (95%)	381 (95%)	19 (5%)	25	14
1	D	399/423 (94%)	379 (95%)	20 (5%)	24	13
All	All	1604/1692 (95%)	1543 (96%)	61 (4%)	33	21

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

Mol	Chain	Res	Type
1	A	24	ASP
1	A	70	VAL

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Mol	Chain	Res	Type
1	A	205	ARG
1	A	266	HIS
1	A	297	TYR
1	A	393	ARG
1	A	398	ARG
1	A	453	ASP
1	B	31	THR
1	B	205	ARG
1	B	266	HIS
1	B	297	TYR
1	B	398	ARG
1	B	406	ARG
1	B	411	LEU
1	B	444	ARG
1	B	446	SER
1	B	482	ARG
1	B	525	ASP
1	B	526	SER
1	B	534	VAL
1	B	537	ARG
1	C	70	VAL
1	C	122	TRP
1	C	126	SER
1	C	143	THR
1	C	160	GLU
1	C	191	ARG
1	C	205	ARG
1	C	266	HIS
1	C	297	TYR
1	C	356	SER
1	C	398	ARG
1	C	458	LEU
1	C	468	LEU
1	C	482	ARG
1	C	489	ARG
1	C	497	SER
1	C	498	LEU
1	C	526	SER
1	C	533	ARG
1	D	70	VAL
1	D	154	VAL
1	D	158	ARG

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Mol	Chain	Res	Type
1	D	160	GLU
1	D	206	LEU
1	D	222	ARG
1	D	263	THR
1	D	266	HIS
1	D	297	TYR
1	D	338	ARG
1	D	398	ARG
1	D	444	ARG
1	D	446	SER
1	D	458	LEU
1	D	468	LEU
1	D	479	LEU
1	D	487	GLN
1	D	491	ARG
1	D	498	LEU
1	D	503	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	211	HIS
1	A	346	ASN
1	A	505	GLN
1	B	96	HIS
1	B	175	HIS
1	B	472	GLN
1	B	505	GLN
1	C	175	HIS
1	C	224	HIS
1	C	472	GLN
1	C	505	GLN
1	D	96	HIS
1	D	175	HIS
1	D	178	ASN
1	D	472	GLN
1	D	505	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	601	-	53,58,58	1.77	10 (18%)	68,89,89	2.47	22 (32%)
2	FAD	D	601	-	53,58,58	1.54	9 (16%)	68,89,89	1.69	13 (19%)

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	601	-	-	5/30/50/50	0/6/6/6
2	FAD	D	601	-	-	11/30/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C1'-C2'	5.80	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C9A-C5X	5.14	1.49	1.41
2	D	601	FAD	C9A-C5X	4.97	1.49	1.41
2	D	601	FAD	O2-C2	3.88	1.31	1.24
2	A	601	FAD	O3B-C3B	3.84	1.52	1.43
2	A	601	FAD	C4X-N5	3.06	1.36	1.30
2	A	601	FAD	C10-N10	2.87	1.43	1.37
2	D	601	FAD	C4X-N5	2.85	1.36	1.30
2	D	601	FAD	C1'-C2'	2.83	1.56	1.52
2	D	601	FAD	C8-C7	2.78	1.47	1.40
2	D	601	FAD	C10-N1	2.70	1.38	1.33
2	A	601	FAD	O2B-C2B	2.54	1.49	1.43
2	D	601	FAD	C5A-C4A	2.40	1.47	1.40
2	D	601	FAD	O4-C4	2.35	1.28	1.23
2	A	601	FAD	C8-C7	2.27	1.46	1.40
2	A	601	FAD	O3'-C3'	2.19	1.48	1.43
2	A	601	FAD	C2'-C3'	2.15	1.57	1.53
2	A	601	FAD	O4-C4	2.06	1.27	1.23
2	D	601	FAD	O4B-C1B	-2.06	1.38	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	C1'-C2'-C3'	8.15	132.58	109.79
2	A	601	FAD	O3'-C3'-C4'	-7.42	90.88	108.81
2	A	601	FAD	O2'-C2'-C3'	-6.78	92.60	109.10
2	D	601	FAD	O3'-C3'-C2'	-5.43	95.70	108.81
2	A	601	FAD	O3'-C3'-C2'	5.22	121.41	108.81
2	D	601	FAD	N3A-C2A-N1A	-5.03	120.81	128.68
2	A	601	FAD	N3A-C2A-N1A	-4.40	121.80	128.68
2	A	601	FAD	O4'-C4'-C5'	4.38	119.77	109.92
2	A	601	FAD	C5'-C4'-C3'	-3.61	105.23	112.20
2	A	601	FAD	C1'-N10-C9A	3.59	126.50	120.51
2	A	601	FAD	C4-C4X-N5	3.53	123.26	118.23
2	D	601	FAD	O2'-C2'-C1'	3.46	118.17	109.80
2	A	601	FAD	O2'-C2'-C1'	-3.34	101.73	109.80
2	A	601	FAD	C4X-C10-N10	3.31	121.33	116.48
2	D	601	FAD	C5'-C4'-C3'	-3.24	105.94	112.20
2	D	601	FAD	O4-C4-C4X	-3.21	118.08	126.60
2	A	601	FAD	C4X-C10-N1	-3.12	117.48	124.73
2	A	601	FAD	C10-N1-C2	3.01	122.92	116.90
2	D	601	FAD	C2A-N1A-C6A	2.91	123.73	118.75
2	A	601	FAD	C9A-N10-C10	-2.83	116.35	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	FAD	C4-C4X-N5	2.79	122.21	118.23
2	A	601	FAD	C2A-N1A-C6A	2.72	123.41	118.75
2	A	601	FAD	C10-C4X-N5	-2.69	119.16	124.86
2	A	601	FAD	C5X-N5-C4X	2.63	122.45	118.07
2	A	601	FAD	C4'-C3'-C2'	-2.63	107.88	113.36
2	A	601	FAD	O4B-C4B-C5B	-2.46	101.28	109.37
2	D	601	FAD	O4B-C1B-C2B	-2.41	103.41	106.93
2	D	601	FAD	O4'-C4'-C3'	2.40	114.94	109.10
2	D	601	FAD	C4A-C5A-N7A	-2.39	106.91	109.40
2	D	601	FAD	C10-N1-C2	2.31	121.52	116.90
2	D	601	FAD	O5'-P-O1P	2.22	117.74	109.07
2	D	601	FAD	C4X-C4-N3	2.18	118.72	113.19
2	A	601	FAD	C5X-C9A-N10	2.09	120.11	117.95
2	A	601	FAD	N6A-C6A-N1A	2.08	122.89	118.57
2	A	601	FAD	O2A-PA-O1A	2.07	122.47	112.24

There are no chirality outliers.

All (16) torsion outliers are listed below:

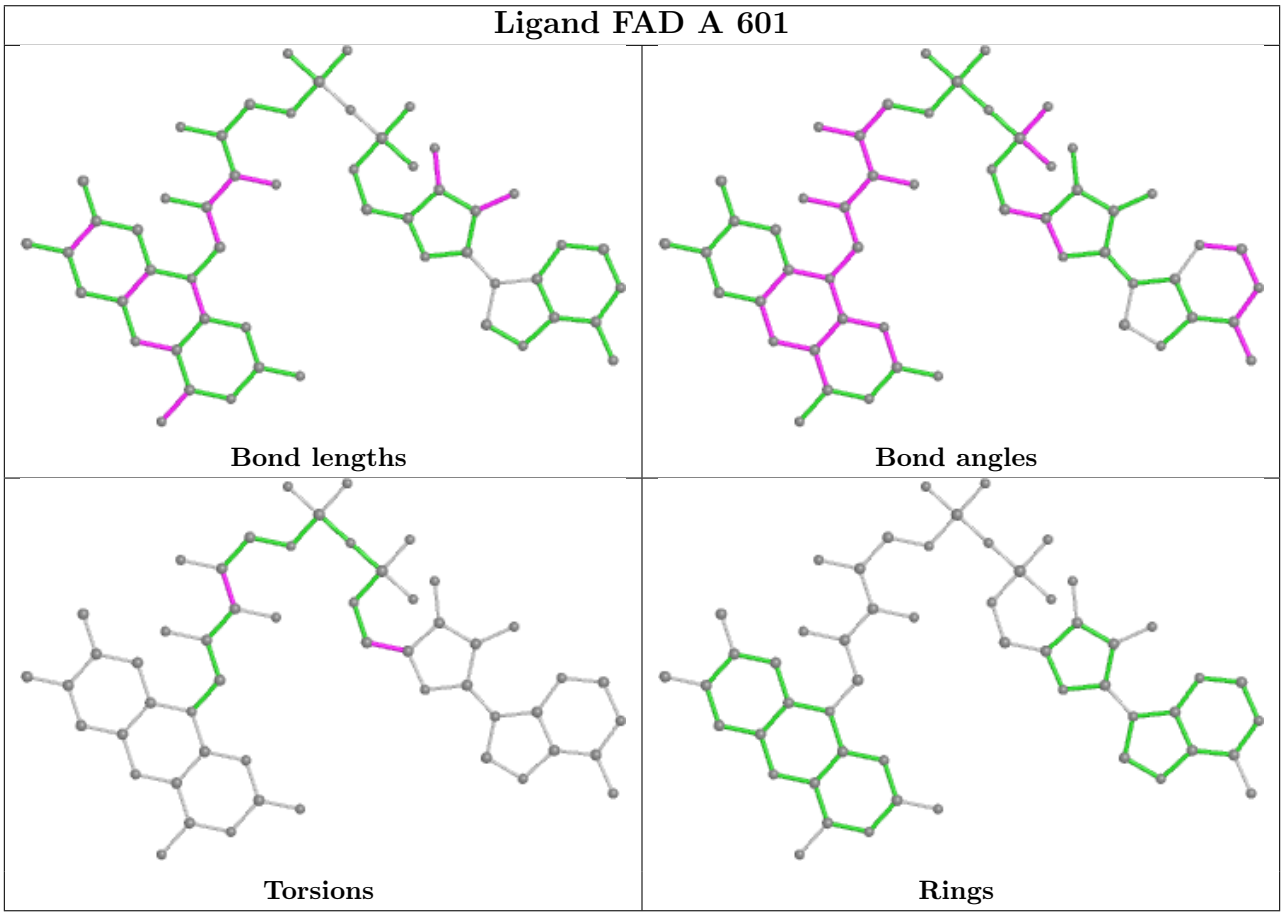
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	N10-C1'-C2'-C3'
2	D	601	FAD	C5'-O5'-P-O1P
2	D	601	FAD	C2'-C3'-C4'-C5'
2	D	601	FAD	O2'-C2'-C3'-O3'
2	D	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	C5'-O5'-P-O3P
2	D	601	FAD	C5'-O5'-P-O2P
2	D	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	O3'-C3'-C4'-C5'
2	D	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B

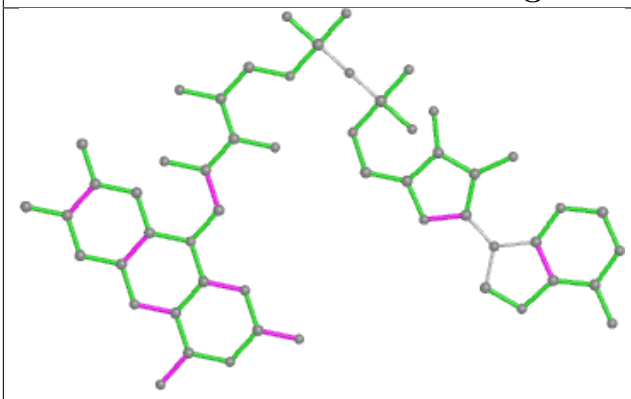
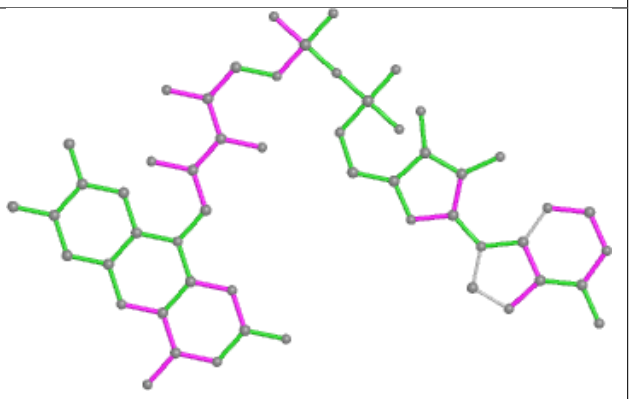
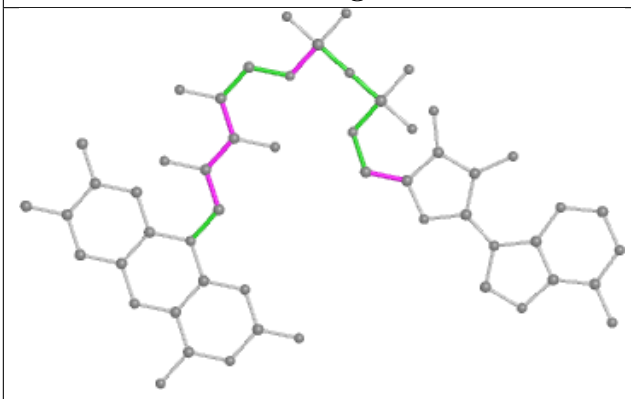
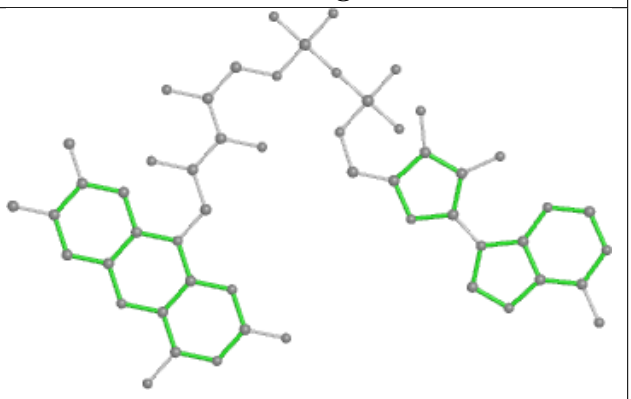
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	14	0
2	D	601	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 D 601	
 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, 95^{th} 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	519/541 (95%)	-0.54	8 (1%)	73	75	22, 32, 55, 116	0
1	B	516/541 (95%)	-0.46	6 (1%)	79	80	20, 31, 57, 96	0
1	C	514/541 (95%)	-0.41	8 (1%)	72	74	21, 34, 70, 106	0
1	D	514/541 (95%)	-0.51	5 (0%)	82	83	20, 31, 57, 106	0
All	All	2063/2164 (95%)	-0.48	27 (1%)	77	79	20, 32, 60, 116	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	VAL	6.0
1	A	24	ASP	5.7
1	A	23	ASP	5.6
1	A	22	ALA	4.3
1	A	21	PRO	4.1
1	C	482	ARG	4.0
1	D	161	GLY	3.8
1	A	160	GLU	3.6
1	B	160	GLU	3.3
1	D	159	GLY	3.2
1	B	378	ARG	3.1
1	D	160	GLU	3.1
1	C	123	GLY	3.1
1	C	378	ARG	2.9
1	A	124	THR	2.9
1	A	378	ARG	2.8
1	B	162	GLY	2.6
1	B	70	VAL	2.5
1	C	539	GLY	2.5
1	C	122	TRP	2.5
1	A	122	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	2.4
1	C	160	GLU	2.4
1	D	378	ARG	2.2
1	B	122	TRP	2.1
1	D	481	PRO	2.1
1	C	71	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

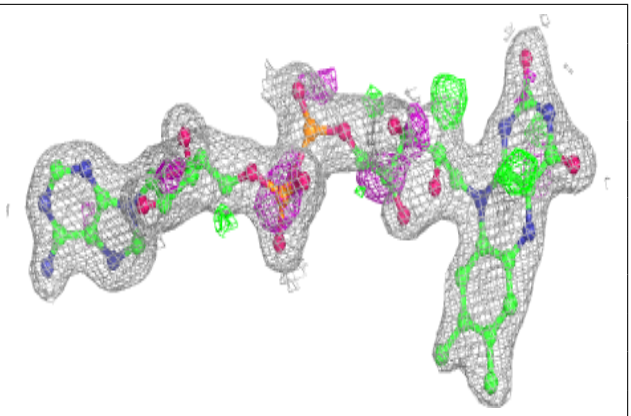
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

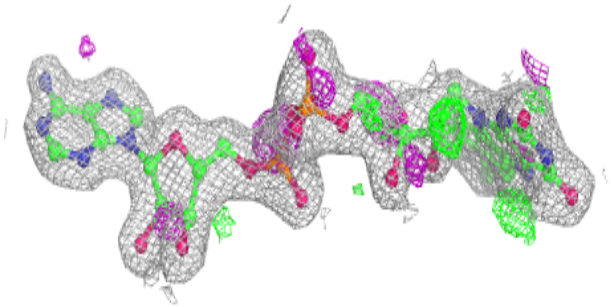
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	601	53/53	0.95	0.11	29,35,49,61	0
2	FAD	D	601	53/53	0.97	0.07	20,28,40,48	0
3	CL	A	602	1/1	0.97	0.18	30,30,30,30	0
3	CL	D	602	1/1	0.99	0.08	30,30,30,30	0

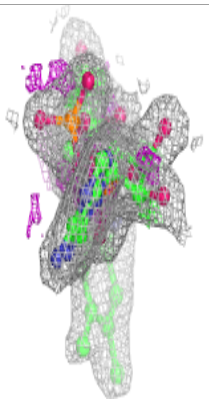
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

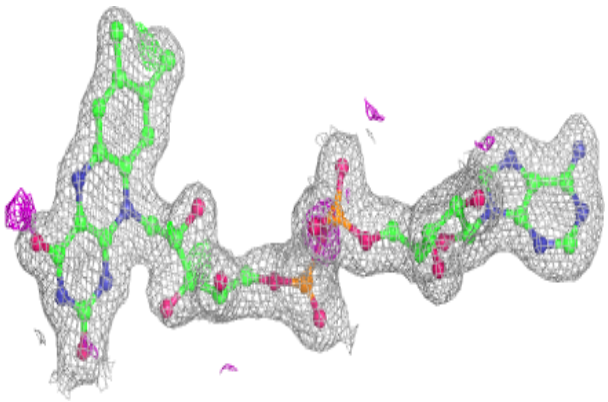


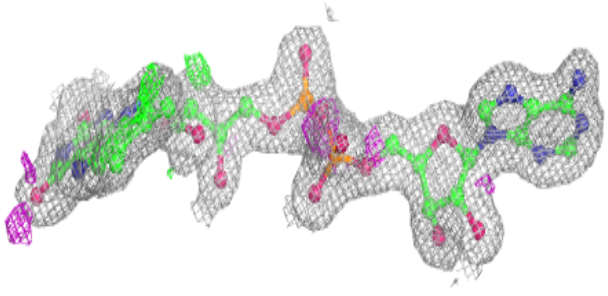


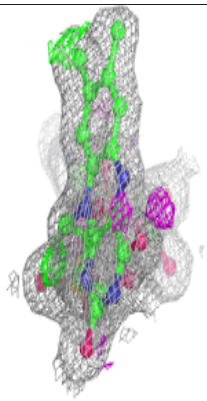


Electron density around FAD D 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.