Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 02:15 pm GMT

PDB ID	:	2XLU
Title	:	Joint-functions of protein residues and NADP(H) in oxygen-activation by flavin-containing monooxygenase: complex with thioNADP
Authors	:	Orru, R.; Fraaije, M.W.; Mattevi, A.
Deposited on	:	2010-07-21
Resolution	:	2.60 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:

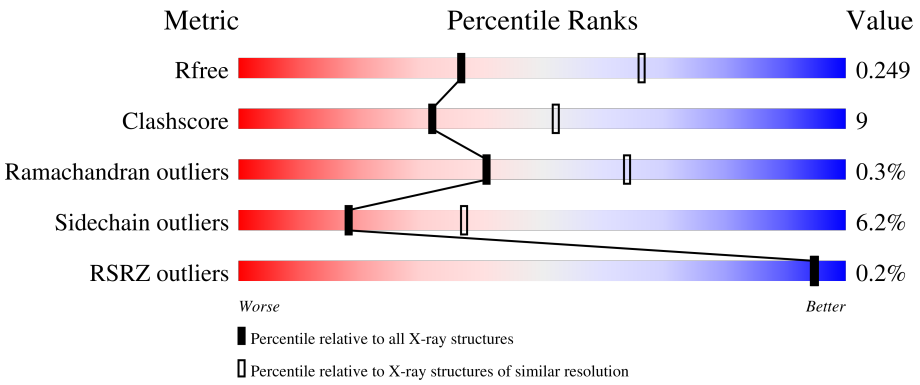
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	461	75% 18% • •
1	B	461	73% 20% • •
1	C	461	75% 20% • •
1	D	461	76% 19% • •

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
5	PEG	A	1453	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15487 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 FLAVIN-CONTAINING MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3659	2347	606	685	21	0	0	0
1	B	445	3651	2343	605	682	21	0	0	0
1	C	445	3651	2343	605	682	21	0	0	0
1	D	446	3659	2347	606	685	21	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q83XK4
A	2	ALA	-	expression tag	UNP Q83XK4
A	3	MET	-	expression tag	UNP Q83XK4
A	4	GLY	-	expression tag	UNP Q83XK4
A	5	SER	-	expression tag	UNP Q83XK4
A	158	ALA	GLU	conflict	UNP Q83XK4
A	159	ALA	GLU	conflict	UNP Q83XK4
B	1	GLY	-	expression tag	UNP Q83XK4
B	2	ALA	-	expression tag	UNP Q83XK4
B	3	MET	-	expression tag	UNP Q83XK4
B	4	GLY	-	expression tag	UNP Q83XK4
B	5	SER	-	expression tag	UNP Q83XK4
B	158	ALA	GLU	conflict	UNP Q83XK4
B	159	ALA	GLU	conflict	UNP Q83XK4
C	1	GLY	-	expression tag	UNP Q83XK4
C	2	ALA	-	expression tag	UNP Q83XK4
C	3	MET	-	expression tag	UNP Q83XK4
C	4	GLY	-	expression tag	UNP Q83XK4
C	5	SER	-	expression tag	UNP Q83XK4
C	158	ALA	GLU	conflict	UNP Q83XK4
C	159	ALA	GLU	conflict	UNP Q83XK4

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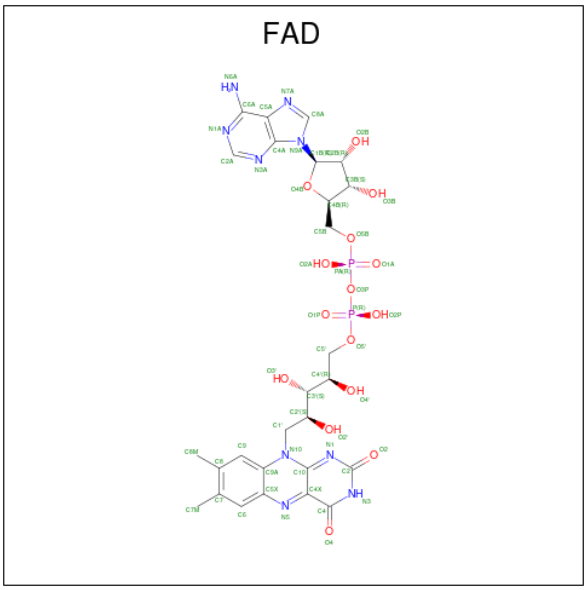
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP Q83XK4
D	2	ALA	-	expression tag	UNP Q83XK4
D	3	MET	-	expression tag	UNP Q83XK4
D	4	GLY	-	expression tag	UNP Q83XK4
D	5	SER	-	expression tag	UNP Q83XK4
D	158	ALA	GLU	conflict	UNP Q83XK4
D	159	ALA	GLU	conflict	UNP Q83XK4

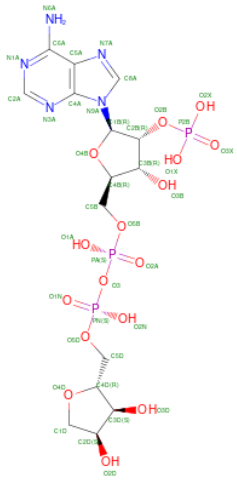
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is [(2R,3R,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3-HYDROXY-4-(PHOSPHONOOXY)TETRAHYDROFURAN-2-YL]METHYL [(2R,3S,4S)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (three-letter code: NA7) (formula: $C_{15}H_{24}N_5O_{16}P_3$).

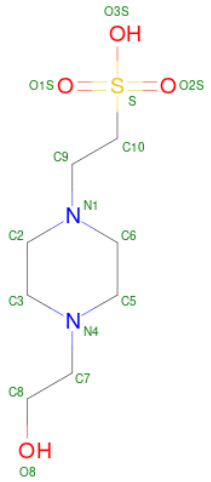
NA7



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	39	15	5	16	3	0	0
			Total	C	N	O	P		
3	B	1	39	15	5	16	3	0	0
			Total	C	N	O	P		
3	C	1	39	15	5	16	3	0	0
			Total	C	N	O	P		
3	D	1	39	15	5	16	3	0	0

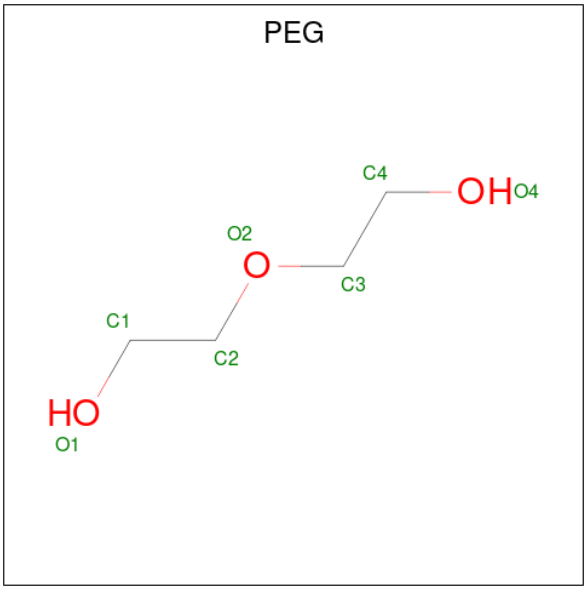
- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

EPE



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0
4	D	1	15	8	2	4	1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	7	4	3		0	0
5	A	1	7	4	3		0	0
5	A	1	7	4	3		0	0
5	B	1	7	4	3		0	0
5	B	1	7	4	3		0	0
5	B	1	7	4	3		0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	99	99	99	0	0
6	B	121	121	121	0	0

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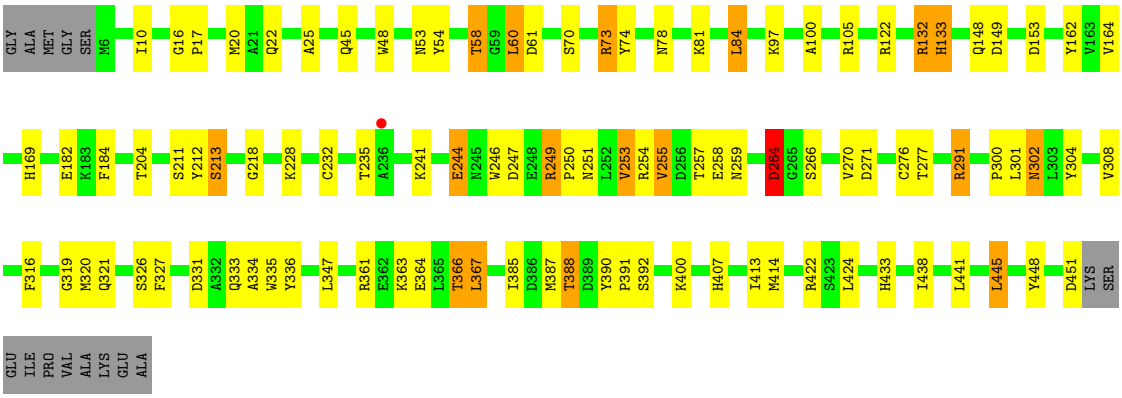
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	C	86	86	86	0	0
			Total	O		
6	D	121	121	121	0	0

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.

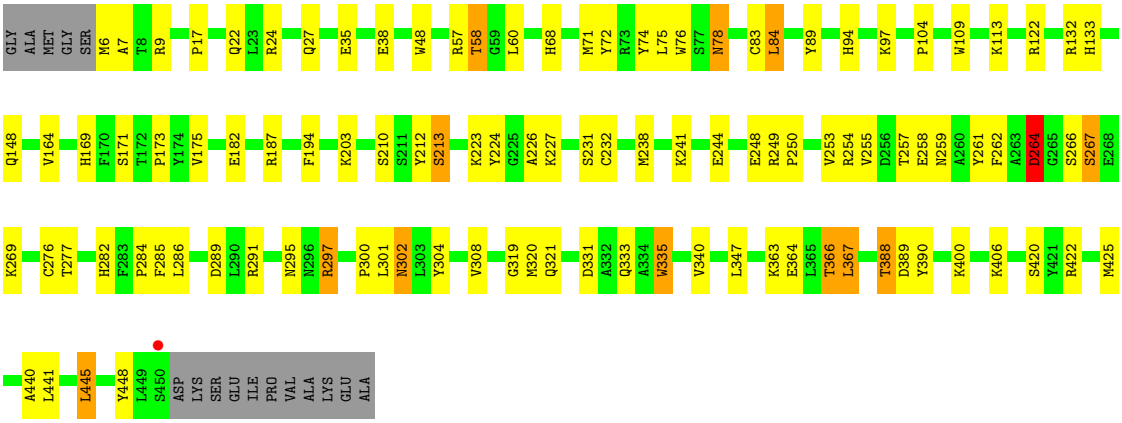
• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain A:



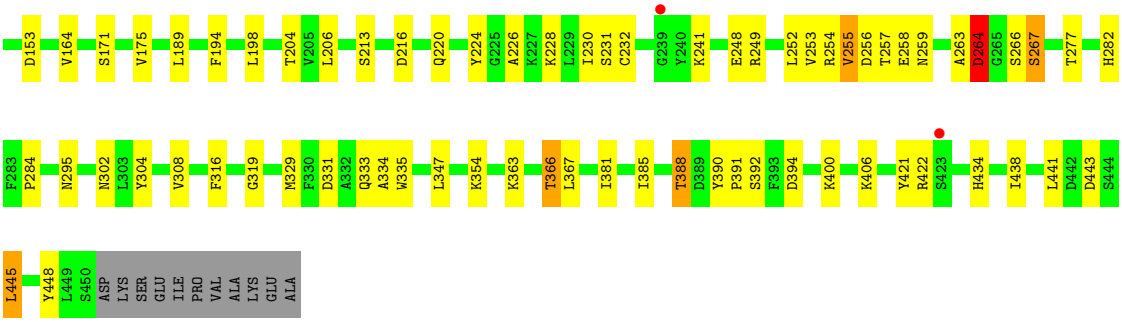
• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain B:



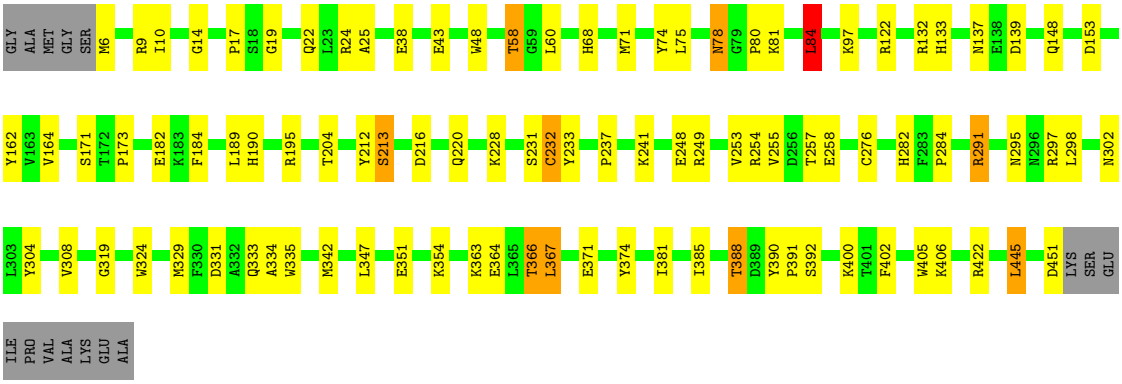
• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain C:



- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	220.68Å 220.68Å 130.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.15 – 2.60 41.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.15-2.60) 99.9 (41.15-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.252 0.208 , 0.249	Depositor DCC
R_{free} test set	5537 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.050 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15487	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA7, PEG, EPE, 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	1.02	4/3773 (0.1%)	0.96	13/5123 (0.3%)
1	B	1.01	2/3765 (0.1%)	0.94	9/5112 (0.2%)
1	C	1.04	0/3765	0.94	6/5112 (0.1%)
1	D	1.00	3/3773 (0.1%)	0.92	7/5123 (0.1%)
All	All	1.02	9/15076 (0.1%)	0.94	35/20470 (0.2%)

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	C	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	GLU	CG-CD	6.93	1.62	1.51
1	A	251	ASN	CB-CG	6.39	1.65	1.51
1	D	182	GLU	CG-CD	6.06	1.61	1.51
1	D	351	GLU	CG-CD	5.59	1.60	1.51
1	A	182	GLU	CG-CD	5.46	1.60	1.51
1	D	232	CYS	CB-SG	-5.28	1.73	1.81
1	B	335	TRP	CB-CG	5.24	1.59	1.50
1	A	316	PHE	CE2-CZ	5.12	1.47	1.37
1	B	83	CYS	CB-SG	-5.08	1.73	1.81

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	122	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	C	445	LEU	CA-CB-CG	9.40	136.93	115.30
1	B	445	LEU	CA-CB-CG	8.15	134.04	115.30
1	A	445	LEU	CA-CB-CG	8.06	133.85	115.30
1	D	445	LEU	CA-CB-CG	7.84	133.34	115.30
1	A	122	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	291	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	361	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	C	32	LYS	CD-CE-NZ	-6.69	96.32	111.70
1	B	84	LEU	CA-CB-CG	6.60	130.49	115.30
1	A	149	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	394	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	122	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	D	122	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	61	ASP	CB-CG-OD1	6.05	123.74	118.30
1	D	195	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	389	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	249	ARG	CB-CG-CD	-5.85	96.40	111.60
1	A	247	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	297	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	B	24	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	291	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	291	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	C	84	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	122	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	73	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	264	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	24	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	84	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	132	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	73	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	187	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	24	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	195	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	289	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	263	ALA	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	3659	0	3446	74	0
1	B	3651	0	3442	65	0
1	C	3651	0	3442	58	0
1	D	3659	0	3446	63	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
2	C	53	0	31	3	0
2	D	53	0	31	4	0
3	A	39	0	20	2	0
3	B	39	0	20	4	0
3	C	39	0	20	2	0
3	D	39	0	20	4	0
4	A	15	0	18	1	0
4	D	15	0	17	0	0
5	A	21	0	30	6	0
5	B	21	0	30	2	0
6	A	99	0	0	9	0
6	B	121	0	0	3	0
6	C	86	0	0	4	0
6	D	121	0	0	8	0
All	All	15487	0	14075	259	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 (259) 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:C:264:ASP:HB3	1:C:266:SER:H	1.17	1.08
1:B:133:HIS:HD2	1:C:133:HIS:HD2	1.08	1.01
1:A:133:HIS:HD2	1:D:133:HIS:HD2	1.02	0.96
1:B:132:ARG:HH21	1:B:148:GLN:HE21	1.12	0.94
1:B:388:THR:HG22	1:B:390:TYR:H	1.33	0.94
1:B:264:ASP:HB3	1:B:266:SER:H	1.37	0.89
1:C:388:THR:HG22	1:C:390:TYR:H	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:HB3	6:A:2059:HOH:O	1.72	0.88
1:B:78:ASN:ND2	6:B:2033:HOH:O	2.07	0.88
1:D:257:THR:HG22	1:D:258:GLU:HG3	1.57	0.87
1:B:132:ARG:HH21	1:B:148:GLN:NE2	1.75	0.85
1:D:58:THR:HB	6:D:2016:HOH:O	1.75	0.85
1:A:133:HIS:HD2	1:D:133:HIS:CD2	1.94	0.84
1:A:319:GLY:H	1:A:333:GLN:HE22	1.24	0.84
1:D:388:THR:HG22	1:D:390:TYR:H	1.42	0.83
1:D:132:ARG:HH21	1:D:148:GLN:HE21	1.24	0.83
1:A:133:HIS:CD2	1:D:133:HIS:HD2	1.93	0.83
1:A:249:ARG:NH1	6:A:2061:HOH:O	2.11	0.82
1:C:388:THR:CG2	1:C:390:TYR:H	1.92	0.81
1:A:264:ASP:HB3	1:A:266:SER:H	1.45	0.80
1:A:407:HIS:HB3	6:A:2089:HOH:O	1.80	0.80
1:D:388:THR:CG2	1:D:390:TYR:H	1.94	0.80
1:A:388:THR:HG22	1:A:390:TYR:H	1.45	0.80
1:A:244:GLU:CB	6:A:2059:HOH:O	2.27	0.79
1:A:132:ARG:HH21	1:A:148:GLN:HE21	1.30	0.78
1:A:258:GLU:HG2	5:A:1453:PEG:H31	1.64	0.78
1:B:388:THR:CG2	1:B:390:TYR:H	1.96	0.77
1:A:249:ARG:HB2	1:A:250:PRO:CD	2.16	0.76
1:B:133:HIS:HD2	1:C:133:HIS:CD2	1.98	0.75
1:A:388:THR:CG2	1:A:390:TYR:H	1.99	0.75
1:B:335:TRP:HB3	1:B:388:THR:HG21	1.67	0.75
1:A:319:GLY:N	1:A:333:GLN:HE22	1.84	0.74
1:B:6:MET:CE	1:B:35:GLU:O	2.35	0.74
1:B:6:MET:HE3	1:B:35:GLU:O	1.87	0.74
1:A:204:THR:HG23	1:A:228:LYS:HB3	1.72	0.70
1:A:132:ARG:HH21	1:A:148:GLN:NE2	1.88	0.70
1:C:206:LEU:HD12	1:C:230:ILE:O	1.91	0.70
1:B:68:HIS:CE1	1:B:171:SER:OG	2.44	0.70
1:D:132:ARG:HH21	1:D:148:GLN:NE2	1.90	0.70
1:B:27:GLN:HE22	5:B:1452:PEG:H42	1.56	0.69
1:C:335:TRP:HB3	1:C:388:THR:HG21	1.74	0.68
1:B:22:GLN:HE21	1:B:164:VAL:HG11	1.59	0.68
1:B:133:HIS:CD2	1:C:133:HIS:HD2	2.00	0.68
1:D:78:ASN:ND2	6:D:2028:HOH:O	2.27	0.66
1:C:319:GLY:H	1:C:333:GLN:HE22	1.44	0.66
1:B:282:HIS:CD2	1:B:284:PRO:HD3	2.31	0.65
1:D:319:GLY:H	1:D:333:GLN:HE22	1.44	0.65
1:A:335:TRP:HB3	1:A:388:THR:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:HH21	1:C:148:GLN:HE21	1.44	0.64
1:A:249:ARG:HB2	1:A:250:PRO:HD3	1.80	0.64
1:B:58:THR:HB	6:C:2048:HOH:O	1.98	0.64
1:C:78:ASN:ND2	6:C:2017:HOH:O	2.30	0.64
1:D:137:ASN:HB3	6:D:2045:HOH:O	1.98	0.63
1:A:58:THR:HB	6:D:2055:HOH:O	1.98	0.63
1:D:6:MET:CE	1:D:342:MET:HG2	2.29	0.63
1:A:319:GLY:H	1:A:333:GLN:NE2	1.96	0.62
1:D:253:VAL:O	1:D:254:ARG:HB3	1.98	0.62
1:D:335:TRP:HB3	1:D:388:THR:HG21	1.81	0.62
1:B:213:SER:HB3	1:B:276:CYS:HB3	1.81	0.62
1:D:132:ARG:NE	6:D:2041:HOH:O	2.28	0.61
1:A:45:GLN:NE2	1:A:53:ASN:HD22	1.98	0.61
1:D:363:LYS:O	1:D:366:THR:HB	2.00	0.61
1:A:232:CYS:HA	1:A:249:ARG:O	2.01	0.60
1:C:198:LEU:HD23	1:C:224:TYR:HB3	1.82	0.60
1:C:319:GLY:N	1:C:333:GLN:HE22	2.00	0.60
1:B:132:ARG:NH2	1:B:148:GLN:HE21	1.93	0.60
1:B:257:THR:HG22	1:B:258:GLU:HG3	1.83	0.60
1:A:363:LYS:O	1:A:366:THR:HB	2.01	0.60
1:D:6:MET:HE2	1:D:342:MET:HG2	1.83	0.59
1:B:291:ARG:NH2	1:C:153:ASP:OD1	2.36	0.58
3:D:501:NA7:O3X	3:D:501:NA7:C1B	2.51	0.58
1:C:22:GLN:HE21	1:C:164:VAL:HG11	1.68	0.58
1:B:388:THR:HG22	1:B:390:TYR:N	2.11	0.58
1:B:363:LYS:O	1:B:366:THR:HB	2.03	0.58
1:A:270:VAL:O	5:A:1453:PEG:C1	2.52	0.57
1:A:301:LEU:O	1:A:302:ASN:CB	2.52	0.57
1:D:385:ILE:HD12	1:D:392:SER:HA	1.87	0.57
1:A:291:ARG:NH2	1:D:153:ASP:OD1	2.37	0.57
1:C:132:ARG:HH21	1:C:148:GLN:NE2	2.02	0.57
1:A:153:ASP:OD1	1:D:291:ARG:NH2	2.38	0.56
1:C:363:LYS:O	1:C:366:THR:HB	2.05	0.56
1:A:244:GLU:HB2	6:A:2059:HOH:O	2.00	0.56
1:C:388:THR:HG22	1:C:390:TYR:N	2.15	0.56
1:D:329:MET:HB2	1:D:381:ILE:HD11	1.87	0.56
1:A:257:THR:HG22	1:A:258:GLU:HG3	1.86	0.56
1:C:68:HIS:CE1	1:C:171:SER:OG	2.58	0.56
1:B:364:GLU:HA	1:B:367:LEU:HD22	1.88	0.56
1:D:173:PRO:HD2	6:D:2049:HOH:O	2.07	0.55
1:D:22:GLN:HE21	1:D:164:VAL:HG11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:PRO:HG2	2:C:500:FAD:H4'	1.90	0.54
1:D:213:SER:HB3	1:D:276:CYS:HB3	1.90	0.53
1:C:204:THR:HG23	1:C:228:LYS:HB3	1.89	0.53
1:D:319:GLY:N	1:D:333:GLN:HE22	2.07	0.53
1:C:264:ASP:HB3	1:C:266:SER:N	2.03	0.53
1:D:402:PHE:O	1:D:405:TRP:HB3	2.09	0.53
1:B:319:GLY:H	1:B:333:GLN:HE22	1.55	0.53
1:A:258:GLU:CG	5:A:1453:PEG:H31	2.38	0.53
1:B:223:LYS:HE2	1:B:224:TYR:CE1	2.44	0.52
1:A:388:THR:HG22	1:A:390:TYR:N	2.20	0.52
1:A:253:VAL:O	1:A:254:ARG:HB3	2.09	0.52
1:B:17:PRO:HG2	2:B:500:FAD:H4'	1.92	0.52
1:C:81:LYS:HA	1:C:84:LEU:HD22	1.91	0.52
1:D:71:MET:HG2	1:D:75:LEU:HD13	1.92	0.51
1:D:304:TYR:HB3	1:D:308:VAL:HB	1.92	0.51
1:D:204:THR:HG23	1:D:228:LYS:HB3	1.91	0.51
3:A:501:NA7:O2N	6:A:2099:HOH:O	2.19	0.51
1:B:223:LYS:NZ	1:B:440:ALA:O	2.24	0.51
1:D:10:ILE:HD12	1:D:162:TYR:HB2	1.93	0.51
1:D:319:GLY:H	1:D:333:GLN:NE2	2.07	0.51
1:A:259:ASN:HD21	5:A:1454:PEG:H32	1.75	0.51
1:A:270:VAL:O	5:A:1453:PEG:H11	2.10	0.51
1:D:216:ASP:O	1:D:220:GLN:HG2	2.11	0.51
1:B:285:PHE:CD1	1:B:286:LEU:HG	2.46	0.50
1:D:139:ASP:HB2	6:D:2045:HOH:O	2.11	0.50
3:D:501:NA7:O3X	3:D:501:NA7:HC1'	2.11	0.50
1:D:17:PRO:HG2	2:D:500:FAD:H4'	1.93	0.50
1:A:184:PHE:HB2	1:A:255:VAL:CG1	2.41	0.50
1:A:73:ARG:HD3	6:A:2051:HOH:O	2.11	0.49
1:B:249:ARG:HB2	1:B:250:PRO:CD	2.42	0.49
1:D:173:PRO:HB3	1:D:190:HIS:CE1	2.48	0.49
1:A:10:ILE:HD12	1:A:162:TYR:HB2	1.94	0.49
1:B:319:GLY:N	1:B:333:GLN:HE22	2.09	0.49
1:C:277:THR:HA	3:C:501:NA7:O4B	2.13	0.49
1:A:326:SER:OG	1:A:327:PHE:N	2.46	0.49
1:C:319:GLY:H	1:C:333:GLN:NE2	2.08	0.49
1:C:304:TYR:HB3	1:C:308:VAL:HB	1.94	0.49
1:D:75:LEU:HD11	2:D:500:FAD:H6	1.94	0.49
1:B:210:SER:HB2	1:B:238:MET:HG3	1.95	0.48
1:A:132:ARG:NH2	1:A:148:GLN:HE21	2.06	0.48
1:B:133:HIS:NE2	6:B:2051:HOH:O	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:NE	6:C:2033:HOH:O	2.43	0.48
1:A:336:TYR:CD1	1:A:387:MET:HE3	2.47	0.48
1:B:232:CYS:HA	1:B:249:ARG:O	2.13	0.48
1:A:304:TYR:HB3	1:A:308:VAL:HB	1.95	0.48
1:C:385:ILE:HD12	1:C:392:SER:HA	1.95	0.48
1:A:271:ASP:HA	5:A:1453:PEG:H12	1.94	0.48
1:B:104:PRO:HD3	1:B:448:TYR:CD1	2.49	0.48
1:C:75:LEU:HD11	2:C:500:FAD:H6	1.96	0.48
1:D:184:PHE:HB2	1:D:255:VAL:CG1	2.43	0.48
1:B:319:GLY:H	1:B:333:GLN:NE2	2.10	0.48
1:A:331:ASP:HB3	1:A:390:TYR:CE1	2.49	0.47
1:D:22:GLN:HA	1:D:334:ALA:HB1	1.96	0.47
1:C:226:ALA:HB2	6:C:2051:HOH:O	2.14	0.47
1:B:71:MET:HG2	1:B:75:LEU:HD13	1.96	0.47
1:C:316:PHE:N	1:C:316:PHE:CD2	2.82	0.47
1:A:45:GLN:HE21	1:A:53:ASN:HD22	1.62	0.47
1:A:364:GLU:HA	1:A:367:LEU:HD22	1.96	0.47
3:B:501:NA7:H51'	3:B:501:NA7:O2A	2.15	0.47
1:B:76:TRP:HA	1:B:104:PRO:HA	1.96	0.47
1:A:81:LYS:O	1:A:84:LEU:HD22	2.15	0.47
1:B:9:ARG:HG3	1:B:38:GLU:HB2	1.97	0.47
1:C:65:GLU:OE2	1:C:132:ARG:NH2	2.46	0.47
1:D:212:TYR:HB2	3:D:501:NA7:H52'	1.96	0.47
1:C:104:PRO:HD3	1:C:448:TYR:CE1	2.50	0.46
1:C:256:ASP:OD1	1:C:259:ASN:N	2.45	0.46
1:D:14:GLY:O	1:D:19:GLY:HA3	2.15	0.46
1:A:22:GLN:HE21	1:A:164:VAL:HG11	1.80	0.46
1:B:261:TYR:N	1:B:261:TYR:CD1	2.84	0.46
1:C:282:HIS:CD2	1:C:284:PRO:HD3	2.50	0.46
1:D:364:GLU:HA	1:D:367:LEU:HD22	1.97	0.46
1:A:424:LEU:N	1:A:424:LEU:HD22	2.30	0.46
1:C:70:SER:HB2	2:C:500:FAD:HM82	1.96	0.46
1:A:390:TYR:CG	1:A:391:PRO:HD2	2.50	0.46
1:B:169:HIS:CD2	1:B:320:MET:HA	2.51	0.46
1:B:182:GLU:OE1	1:B:182:GLU:N	2.32	0.46
1:B:295:ASN:OD1	1:B:297:ARG:HD2	2.16	0.45
1:C:231:SER:HB2	1:C:248:GLU:HG2	1.98	0.45
1:C:331:ASP:HB3	1:C:390:TYR:CE1	2.50	0.45
1:B:109:TRP:CD2	1:B:113:LYS:HE2	2.51	0.45
1:A:413:ILE:HG23	1:A:414:MET:HG2	1.97	0.45
1:A:301:LEU:O	1:A:302:ASN:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:SER:HB2	1:B:248:GLU:HG2	1.98	0.45
3:D:501:NA7:O2A	3:D:501:NA7:H51'	2.17	0.45
1:B:262:PHE:CD2	1:B:262:PHE:N	2.84	0.45
1:C:253:VAL:O	1:C:254:ARG:HB3	2.16	0.45
1:B:212:TYR:HB2	3:B:501:NA7:H52'	1.98	0.45
1:A:169:HIS:CD2	1:A:320:MET:HA	2.51	0.45
1:A:277:THR:HA	3:A:501:NA7:O4B	2.17	0.45
1:B:173:PRO:HB2	1:B:175:VAL:CG2	2.47	0.45
1:B:253:VAL:O	1:B:254:ARG:HB3	2.17	0.44
1:C:72:TYR:CD1	1:C:194:PHE:HD2	2.35	0.44
3:B:501:NA7:C1B	3:B:501:NA7:O3X	2.64	0.44
1:C:45:GLN:NE2	1:C:53:ASN:HD22	2.16	0.44
1:B:57:ARG:HH12	1:C:175:VAL:HB	1.82	0.44
1:A:213:SER:HB3	1:A:276:CYS:HB3	1.99	0.44
1:C:9:ARG:HG3	1:C:38:GLU:HB2	1.98	0.44
1:C:257:THR:HG22	1:C:258:GLU:HG3	1.99	0.44
1:B:72:TYR:CD1	1:B:194:PHE:HD2	2.35	0.44
1:D:298:LEU:HD21	1:D:324:TRP:CD1	2.52	0.44
1:A:211:SER:OG	1:A:212:TYR:N	2.43	0.44
1:A:100:ALA:HB3	1:A:448:TYR:OH	2.18	0.43
2:D:500:FAD:O2'	2:D:500:FAD:C5'	2.66	0.43
1:B:335:TRP:CB	1:B:388:THR:HG21	2.43	0.43
3:C:501:NA7:C1B	3:C:501:NA7:O3X	2.64	0.43
1:D:371:GLU:HA	1:D:374:TYR:CZ	2.54	0.43
1:A:385:ILE:HD12	1:A:392:SER:HA	2.00	0.43
1:A:16:GLY:O	1:A:20:MET:HG3	2.19	0.43
1:B:7:ALA:O	6:B:2001:HOH:O	2.22	0.43
1:D:43:GLU:OE2	2:D:500:FAD:O2B	2.36	0.43
1:D:331:ASP:HB3	1:D:390:TYR:CE1	2.54	0.43
1:D:388:THR:HG22	1:D:390:TYR:N	2.21	0.43
1:C:6:MET:HE3	1:C:37:PRO:HD3	2.01	0.43
1:C:103:PRO:HA	1:C:104:PRO:HD3	1.95	0.43
1:A:218:GLY:HA3	1:A:246:TRP:CH2	2.53	0.43
1:B:104:PRO:HD3	1:B:448:TYR:CE1	2.54	0.43
1:B:89:TYR:CE2	1:B:94:HIS:HB2	2.54	0.42
1:D:388:THR:HG23	1:D:390:TYR:H	1.76	0.42
1:A:17:PRO:HG2	2:A:500:FAD:H4'	2.01	0.42
1:C:252:LEU:HD11	1:C:255:VAL:HG23	2.01	0.42
1:B:285:PHE:CE1	1:B:286:LEU:HG	2.55	0.42
1:C:22:GLN:HA	1:C:334:ALA:HB1	2.00	0.42
1:C:102:TYR:OH	1:C:421:TYR:OH	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ARG:CD	6:D:2041:HOH:O	2.65	0.42
1:A:390:TYR:HA	1:A:391:PRO:HD3	1.64	0.42
1:B:331:ASP:HB3	1:B:390:TYR:CE1	2.55	0.42
1:A:22:GLN:HA	1:A:334:ALA:HB1	2.01	0.42
1:D:81:LYS:HA	1:D:84:LEU:HD22	2.02	0.42
1:D:231:SER:HB2	1:D:248:GLU:HG2	2.02	0.42
1:C:72:TYR:CZ	1:C:75:LEU:HD12	2.55	0.42
1:A:84:LEU:HD23	1:A:84:LEU:C	2.40	0.42
1:A:424:LEU:HD22	1:A:424:LEU:H	1.84	0.42
1:C:438:ILE:O	1:C:438:ILE:HG13	2.20	0.42
1:A:300:PRO:HD2	1:A:321:GLN:HG3	2.02	0.41
1:C:390:TYR:HA	1:C:391:PRO:HD3	1.85	0.41
1:A:70:SER:HB2	2:A:500:FAD:HM82	2.02	0.41
1:A:448:TYR:HB2	6:A:2096:HOH:O	2.20	0.41
1:B:304:TYR:HB3	1:B:308:VAL:HB	2.02	0.41
1:C:232:CYS:HA	1:C:249:ARG:O	2.19	0.41
1:A:100:ALA:CB	1:A:433:HIS:HB2	2.51	0.41
1:A:249:ARG:CZ	6:A:2061:HOH:O	2.62	0.41
1:B:241:LYS:HD2	1:B:241:LYS:HA	1.77	0.41
1:D:282:HIS:CD2	1:D:284:PRO:HD3	2.56	0.41
1:C:74:TYR:HA	1:C:443:ASP:HB3	2.02	0.41
1:D:6:MET:HE1	1:D:342:MET:HG2	2.00	0.41
1:A:438:ILE:O	1:A:438:ILE:HG13	2.21	0.41
1:B:226:ALA:O	1:B:227:LYS:C	2.58	0.41
1:B:301:LEU:O	1:B:302:ASN:CB	2.67	0.41
3:B:501:NA7:O3X	3:B:501:NA7:HC1'	2.21	0.41
1:D:241:LYS:HD2	1:D:241:LYS:HA	1.86	0.41
1:C:329:MET:HB2	1:C:381:ILE:HD11	2.02	0.41
1:D:233:TYR:CE2	1:D:237:PRO:HD3	2.56	0.41
1:D:295:ASN:OD1	1:D:297:ARG:HD2	2.21	0.41
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.85	0.41
1:B:253:VAL:HG22	1:B:261:TYR:O	2.19	0.40
1:D:80:PRO:HD3	1:D:405:TRP:CD1	2.56	0.40
1:D:184:PHE:HB2	1:D:255:VAL:HG11	2.02	0.40
1:A:54:TYR:HB2	1:A:105:ARG:CZ	2.52	0.40
1:D:9:ARG:HG3	1:D:38:GLU:HB2	2.03	0.40
4:A:1452:EPE:H82	1:C:295:ASN:HB3	2.02	0.40
1:D:390:TYR:HA	1:D:391:PRO:HD3	1.85	0.40
1:B:300:PRO:HD2	1:B:321:GLN:HG3	2.03	0.40
1:B:425:MET:O	5:B:1451:PEG:H41	2.21	0.40
1:C:76:TRP:O	1:C:77:SER:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:HIS:CE1	1:D:171:SER:OG	2.74	0.40
1:A:25:ALA:HB2	1:A:335:TRP:CE3	2.57	0.40
1:B:255:VAL:HA	1:B:259:ASN:O	2.21	0.40
1:C:216:ASP:O	1:C:220:GLN:HG2	2.21	0.40
1:D:25:ALA:HB2	1:D:335:TRP:CE3	2.55	0.40
1:D:232:CYS:HA	1:D:249:ARG:O	2.22	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	444/461 (96%)	418 (94%)	26 (6%)	0	100	100
1	B	443/461 (96%)	416 (94%)	25 (6%)	2 (0%)	29	52
1	C	443/461 (96%)	408 (92%)	32 (7%)	3 (1%)	22	43
1	D	444/461 (96%)	421 (95%)	23 (5%)	0	100	100
All	All	1774/1844 (96%)	1663 (94%)	106 (6%)	5 (0%)	41	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	ASP
1	B	267	SER
1	C	264	ASP
1	C	77	SER
1	C	267	SER

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	387/397 (98%)	363 (94%)	24 (6%)	18	37
1	B	386/397 (97%)	360 (93%)	26 (7%)	16	33
1	C	386/397 (97%)	360 (93%)	26 (7%)	16	33
1	D	387/397 (98%)	367 (95%)	20 (5%)	23	46
All	All	1546/1588 (97%)	1450 (94%)	96 (6%)	18	37

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	TRP
1	A	58	THR
1	A	60	LEU
1	A	74	TYR
1	A	78	ASN
1	A	84	LEU
1	A	97	LYS
1	A	133	HIS
1	A	213	SER
1	A	235	THR
1	A	241	LYS
1	A	253	VAL
1	A	255	VAL
1	A	264	ASP
1	A	302	ASN
1	A	347	LEU
1	A	366	THR
1	A	367	LEU
1	A	388	THR
1	A	400	LYS
1	A	422	ARG
1	A	441	LEU
1	A	445	LEU
1	A	451	ASP

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Mol	Chain	Res	Type
1	B	48	TRP
1	B	58	THR
1	B	60	LEU
1	B	74	TYR
1	B	78	ASN
1	B	84	LEU
1	B	97	LYS
1	B	203	LYS
1	B	213	SER
1	B	244	GLU
1	B	264	ASP
1	B	267	SER
1	B	269	LYS
1	B	277	THR
1	B	302	ASN
1	B	340	VAL
1	B	347	LEU
1	B	366	THR
1	B	367	LEU
1	B	388	THR
1	B	400	LYS
1	B	406	LYS
1	B	420	SER
1	B	422	ARG
1	B	441	LEU
1	B	445	LEU
1	C	48	TRP
1	C	58	THR
1	C	60	LEU
1	C	74	TYR
1	C	78	ASN
1	C	84	LEU
1	C	97	LYS
1	C	133	HIS
1	C	189	LEU
1	C	213	SER
1	C	241	LYS
1	C	255	VAL
1	C	264	ASP
1	C	267	SER
1	C	302	ASN
1	C	347	LEU

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Mol	Chain	Res	Type
1	C	354	LYS
1	C	366	THR
1	C	367	LEU
1	C	388	THR
1	C	400	LYS
1	C	406	LYS
1	C	422	ARG
1	C	434	HIS
1	C	441	LEU
1	C	445	LEU
1	D	48	TRP
1	D	58	THR
1	D	60	LEU
1	D	74	TYR
1	D	78	ASN
1	D	84	LEU
1	D	97	LYS
1	D	189	LEU
1	D	213	SER
1	D	302	ASN
1	D	347	LEU
1	D	354	LYS
1	D	366	THR
1	D	367	LEU
1	D	388	THR
1	D	400	LYS
1	D	406	LYS
1	D	422	ARG
1	D	445	LEU
1	D	451	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	45	GLN
1	A	133	HIS
1	A	148	GLN
1	A	282	HIS
1	A	302	ASN
1	A	333	GLN
1	A	433	HIS

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Mol	Chain	Res	Type
1	B	22	GLN
1	B	27	GLN
1	B	45	GLN
1	B	78	ASN
1	B	148	GLN
1	B	282	HIS
1	B	333	GLN
1	B	419	HIS
1	C	22	GLN
1	C	45	GLN
1	C	78	ASN
1	C	148	GLN
1	C	302	ASN
1	C	333	GLN
1	C	419	HIS
1	D	22	GLN
1	D	45	GLN
1	D	133	HIS
1	D	148	GLN
1	D	302	ASN
1	D	333	GLN

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)

16 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	NA7	A	501	-	36,42,42	1.34	6 (16%)	43,65,65	2.02	14 (32%)
2	FAD	A	500	-	53,58,58	1.30	6 (11%)	68,89,89	1.67	16 (23%)
3	NA7	B	501	-	36,42,42	1.19	3 (8%)	43,65,65	1.95	11 (25%)
5	PEG	A	1454	-	6,6,6	0.89	0	5,5,5	1.16	1 (20%)
3	NA7	D	501	-	36,42,42	1.08	2 (5%)	43,65,65	2.25	14 (32%)
2	FAD	B	500	-	53,58,58	1.24	3 (5%)	68,89,89	1.58	12 (17%)
5	PEG	A	1453	-	6,6,6	0.50	0	5,5,5	1.90	1 (20%)
3	NA7	C	501	-	36,42,42	1.17	2 (5%)	43,65,65	2.23	12 (27%)
5	PEG	B	1453	-	6,6,6	0.58	0	5,5,5	0.69	0
5	PEG	B	1451	-	6,6,6	1.01	0	5,5,5	0.84	0
4	EPE	D	1452	-	15,15,15	1.29	1 (6%)	18,20,20	3.15	11 (61%)
2	FAD	D	500	-	53,58,58	1.33	3 (5%)	68,89,89	1.49	9 (13%)
5	PEG	B	1452	-	6,6,6	0.83	0	5,5,5	0.73	0
2	FAD	C	500	-	53,58,58	1.23	4 (7%)	68,89,89	1.66	18 (26%)
5	PEG	A	1455	-	6,6,6	0.62	0	5,5,5	0.71	0
4	EPE	A	1452	-	15,15,15	1.42	1 (6%)	18,20,20	2.46	6 (33%)

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	NA7	A	501	-	-	5/23/56/56	0/4/4/4
2	FAD	A	500	-	-	3/30/50/50	0/6/6/6
3	NA7	B	501	-	-	6/23/56/56	0/4/4/4
5	PEG	A	1454	-	-	3/4/4/4	-
3	NA7	D	501	-	-	7/23/56/56	0/4/4/4
2	FAD	B	500	-	-	7/30/50/50	0/6/6/6
5	PEG	A	1453	-	-	2/4/4/4	-
3	NA7	C	501	-	-	9/23/56/56	0/4/4/4
5	PEG	B	1453	-	-	3/4/4/4	-
5	PEG	B	1451	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	D	1452	-	-	5/9/19/19	0/1/1/1
2	FAD	D	500	-	-	3/30/50/50	0/6/6/6
5	PEG	B	1452	-	-	3/4/4/4	-
2	FAD	C	500	-	-	6/30/50/50	0/6/6/6
5	PEG	A	1455	-	-	3/4/4/4	-
4	EPE	A	1452	-	-	3/9/19/19	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1452	EPE	C10-S	4.91	1.84	1.77
2	C	500	FAD	C4X-N5	4.66	1.39	1.30
4	D	1452	EPE	C10-S	4.59	1.84	1.77
2	C	500	FAD	C2A-N3A	4.44	1.39	1.32
2	A	500	FAD	C2A-N3A	4.28	1.39	1.32
2	A	500	FAD	C4X-N5	3.99	1.38	1.30
2	D	500	FAD	C4X-N5	3.92	1.38	1.30
2	B	500	FAD	C4X-N5	3.88	1.38	1.30
2	B	500	FAD	C2A-N3A	3.77	1.38	1.32
2	D	500	FAD	C10-N1	3.70	1.40	1.33
2	D	500	FAD	C2A-N3A	3.56	1.37	1.32
3	C	501	NA7	O4B-C1B	3.52	1.46	1.41
3	B	501	NA7	PA-O2A	3.32	1.62	1.50
3	A	501	NA7	PA-O2A	3.13	1.62	1.50
3	A	501	NA7	O4B-C1B	3.01	1.45	1.41
2	B	500	FAD	C10-N1	2.99	1.39	1.33
3	D	501	NA7	PA-O2A	2.94	1.61	1.50
3	C	501	NA7	PA-O2A	2.90	1.61	1.50
3	A	501	NA7	C2A-N3A	2.73	1.36	1.32
3	B	501	NA7	O4B-C1B	2.64	1.44	1.41
2	A	500	FAD	C10-N1	2.62	1.38	1.33
2	C	500	FAD	C10-N1	2.57	1.38	1.33
3	B	501	NA7	C2A-N3A	2.45	1.36	1.32
3	D	501	NA7	C2A-N3A	2.45	1.36	1.32
2	A	500	FAD	C8M-C8	-2.36	1.46	1.51
3	A	501	NA7	P2B-O1X	2.28	1.63	1.54
3	A	501	NA7	C1D-C2D	2.25	1.55	1.51
2	A	500	FAD	C4-N3	-2.17	1.34	1.38
2	C	500	FAD	C1'-N10	2.13	1.53	1.48
3	A	501	NA7	O4D-C1D	2.12	1.48	1.43
2	A	500	FAD	C4X-C10	-2.01	1.38	1.44

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	NA7	O2B-P2B-O3X	-7.69	79.73	109.39
4	D	1452	EPE	O2S-S-C10	7.29	115.69	106.92
2	A	500	FAD	N3A-C2A-N1A	-6.66	118.27	128.68
3	C	501	NA7	O2B-P2B-O3X	-6.47	84.41	109.39
2	D	500	FAD	N3A-C2A-N1A	-6.19	119.01	128.68
3	A	501	NA7	N3A-C2A-N1A	-5.93	119.40	128.68
4	A	1452	EPE	O1S-S-C10	5.91	114.03	106.92
3	B	501	NA7	O2B-P2B-O3X	-5.67	87.49	109.39
3	C	501	NA7	O2B-C2B-C1B	5.67	130.50	110.10
4	D	1452	EPE	O3S-S-C10	5.63	114.87	105.77
3	D	501	NA7	O2B-C2B-C1B	5.15	128.63	110.10
3	D	501	NA7	O4B-C1B-C2B	-5.14	97.67	106.59
3	C	501	NA7	O4B-C1B-C2B	-5.05	97.83	106.59
2	B	500	FAD	N3A-C2A-N1A	-4.77	121.22	128.68
2	C	500	FAD	N3A-C2A-N1A	-4.74	121.28	128.68
3	C	501	NA7	N3A-C2A-N1A	-4.68	121.37	128.68
4	A	1452	EPE	C5-N4-C3	4.56	119.09	108.83
3	A	501	NA7	O4B-C1B-C2B	-4.17	99.36	106.59
3	B	501	NA7	O4B-C1B-C2B	-4.14	99.41	106.59
3	B	501	NA7	N3A-C2A-N1A	-4.07	122.32	128.68
3	A	501	NA7	O2B-C2B-C1B	4.00	124.50	110.10
4	A	1452	EPE	C7-N4-C5	3.86	121.10	111.23
3	A	501	NA7	C2B-C3B-C4B	-3.81	93.73	101.99
4	D	1452	EPE	C5-N4-C3	3.76	117.29	108.83
4	D	1452	EPE	C7-N4-C5	3.71	120.72	111.23
2	B	500	FAD	C1'-N10-C9A	3.68	126.65	120.51
2	A	500	FAD	C4X-C4-N3	3.63	122.42	113.19
2	A	500	FAD	O2'-C2'-C1'	-3.61	101.06	109.80
2	C	500	FAD	C5X-C9A-N10	3.60	121.67	117.95
3	C	501	NA7	O2X-P2B-O2B	3.57	121.97	105.99
2	B	500	FAD	C4A-C5A-N7A	-3.50	105.76	109.40
3	B	501	NA7	O2X-P2B-O2B	3.47	121.52	105.99
3	B	501	NA7	O3D-C3D-C4D	-3.46	101.05	111.05
5	A	1453	PEG	O4-C4-C3	-3.45	91.78	111.81
3	C	501	NA7	PN-O3-PA	-3.41	121.13	132.83
2	B	500	FAD	O4-C4-C4X	-3.37	117.65	126.60
3	C	501	NA7	O2D-C2D-C3D	3.36	117.63	111.27
4	A	1452	EPE	C7-N4-C3	3.33	119.75	111.23
3	B	501	NA7	O2B-C2B-C1B	3.33	122.09	110.10
4	D	1452	EPE	C5-C6-N1	3.33	117.47	110.64
3	B	501	NA7	C1B-N9A-C4A	-3.31	120.83	126.64
2	C	500	FAD	C1'-N10-C9A	3.29	126.00	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	FAD	C9A-C5X-N5	-3.23	118.93	122.43
2	B	500	FAD	C4X-C10-N10	3.21	121.17	116.48
2	B	500	FAD	C4X-C4-N3	3.09	121.03	113.19
3	A	501	NA7	C5B-C4B-C3B	-3.08	103.66	115.18
2	D	500	FAD	C4X-C4-N3	3.07	120.98	113.19
2	A	500	FAD	C9A-C5X-N5	-3.04	119.12	122.43
4	D	1452	EPE	C6-C5-N4	3.03	116.86	110.64
2	C	500	FAD	C4A-C5A-N7A	-3.02	106.25	109.40
4	D	1452	EPE	C3-C2-N1	2.98	116.75	110.64
2	A	500	FAD	C4-N3-C2	-2.98	120.14	125.64
2	C	500	FAD	C4X-C10-N10	2.96	120.81	116.48
2	B	500	FAD	C4-N3-C2	-2.94	120.20	125.64
4	A	1452	EPE	O2S-S-O1S	-2.93	103.80	113.95
3	A	501	NA7	O2D-C2D-C3D	2.85	116.66	111.27
3	D	501	NA7	O2N-PN-O5D	-2.85	94.52	107.75
3	A	501	NA7	O4D-C4D-C3D	-2.84	102.19	104.70
3	D	501	NA7	C5B-C4B-C3B	-2.83	104.58	115.18
4	D	1452	EPE	C7-N4-C3	2.82	118.44	111.23
3	D	501	NA7	N3A-C2A-N1A	-2.79	124.31	128.68
3	A	501	NA7	O5B-C5B-C4B	-2.79	99.39	108.99
4	D	1452	EPE	C6-N1-C2	2.79	115.10	108.83
2	A	500	FAD	O5'-C5'-C4'	-2.76	102.00	109.36
2	C	500	FAD	C4-N3-C2	-2.73	120.59	125.64
3	B	501	NA7	O2B-C2B-C3B	2.73	121.58	111.68
3	D	501	NA7	O2D-C2D-C3D	2.69	116.37	111.27
2	C	500	FAD	C4X-C4-N3	2.69	120.03	113.19
3	D	501	NA7	O2X-P2B-O3X	2.68	121.17	110.68
2	A	500	FAD	O4-C4-N3	-2.67	115.00	120.12
4	D	1452	EPE	O3S-S-O2S	-2.66	104.77	111.27
2	A	500	FAD	C4X-C10-N10	2.58	120.26	116.48
3	A	501	NA7	O4B-C4B-C3B	2.54	110.14	105.11
2	C	500	FAD	C10-N1-C2	2.54	121.98	116.90
3	D	501	NA7	O5D-PN-O1N	2.54	118.98	109.07
2	D	500	FAD	O5'-C5'-C4'	-2.54	102.59	109.36
2	C	500	FAD	O4-C4-C4X	-2.52	119.92	126.60
3	A	501	NA7	C4A-C5A-N7A	-2.51	106.78	109.40
2	A	500	FAD	C4X-C10-N1	-2.50	118.93	124.73
3	D	501	NA7	C2B-C3B-C4B	-2.49	96.58	101.99
2	D	500	FAD	C5X-C9A-N10	2.49	120.52	117.95
2	D	500	FAD	C9A-C5X-N5	-2.47	119.75	122.43
2	B	500	FAD	P-O3P-PA	-2.46	124.37	132.83
3	D	501	NA7	O1X-P2B-O2B	2.46	117.03	105.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	FAD	C9A-C5X-N5	-2.46	119.76	122.43
3	B	501	NA7	C5B-C4B-C3B	-2.42	106.13	115.18
3	C	501	NA7	C2A-N1A-C6A	2.38	122.82	118.75
2	B	500	FAD	C4X-C10-N1	-2.36	119.26	124.73
4	A	1452	EPE	C6-C5-N4	2.33	115.43	110.64
3	B	501	NA7	O5D-PN-O1N	2.33	118.17	109.07
3	A	501	NA7	C1D-C2D-C3D	2.33	105.18	101.63
3	D	501	NA7	O4D-C4D-C3D	2.32	106.76	104.70
2	A	500	FAD	C5X-C9A-N10	2.31	120.34	117.95
2	D	500	FAD	O4-C4-C4X	-2.29	120.52	126.60
2	C	500	FAD	C4X-C10-N1	-2.29	119.42	124.73
3	C	501	NA7	C5B-C4B-C3B	-2.28	106.64	115.18
2	C	500	FAD	C1B-N9A-C4A	-2.27	122.65	126.64
3	D	501	NA7	O2X-P2B-O2B	2.25	116.09	105.99
2	A	500	FAD	C4-C4X-N5	2.25	121.44	118.23
2	B	500	FAD	O4B-C1B-C2B	-2.24	103.65	106.93
2	A	500	FAD	C10-C4X-N5	-2.23	120.12	124.86
3	B	501	NA7	C4A-C5A-N7A	-2.21	107.09	109.40
2	C	500	FAD	C9A-C9-C8	2.20	123.73	119.30
2	C	500	FAD	C9-C9A-C5X	-2.18	116.00	120.11
3	A	501	NA7	C1B-N9A-C4A	-2.17	122.83	126.64
5	A	1454	PEG	O2-C3-C4	2.17	119.59	110.07
2	D	500	FAD	C4-N3-C2	-2.16	121.65	125.64
2	A	500	FAD	P-O3P-PA	-2.16	125.43	132.83
2	A	500	FAD	C4A-C5A-N7A	-2.12	107.19	109.40
2	C	500	FAD	P-O3P-PA	-2.12	125.56	132.83
3	C	501	NA7	C1D-C2D-C3D	-2.11	98.42	101.63
2	A	500	FAD	C10-N1-C2	2.10	121.09	116.90
2	C	500	FAD	C4'-C3'-C2'	-2.10	109.00	113.36
2	C	500	FAD	C10-C4X-N5	-2.09	120.43	124.86
3	C	501	NA7	O2D-C2D-C1D	-2.08	104.75	110.97
4	D	1452	EPE	C9-N1-C6	-2.07	105.94	111.23
3	D	501	NA7	O2N-PN-O1N	2.07	122.45	112.24
2	A	500	FAD	C2A-N1A-C6A	2.06	122.28	118.75
3	C	501	NA7	O4D-C4D-C3D	-2.06	102.88	104.70
3	A	501	NA7	O3D-C3D-C4D	-2.06	105.10	111.05
2	D	500	FAD	C4X-C10-N1	-2.04	120.00	124.73
2	C	500	FAD	O2'-C2'-C3'	-2.03	104.16	109.10
2	B	500	FAD	C5X-C9A-N10	2.01	120.03	117.95
2	D	500	FAD	C10-N1-C2	2.01	120.92	116.90
3	A	501	NA7	O1A-PA-O5B	-2.00	98.44	107.75

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FAD	N10-C1'-C2'-O2'
2	A	500	FAD	N10-C1'-C2'-C3'
2	B	500	FAD	N10-C1'-C2'-O2'
2	B	500	FAD	N10-C1'-C2'-C3'
2	C	500	FAD	N10-C1'-C2'-O2'
2	C	500	FAD	N10-C1'-C2'-C3'
2	D	500	FAD	N10-C1'-C2'-O2'
2	D	500	FAD	N10-C1'-C2'-C3'
3	A	501	NA7	C3D-C4D-C5D-O5D
3	C	501	NA7	C5B-O5B-PA-O3
3	C	501	NA7	C5D-O5D-PN-O3
4	A	1452	EPE	C10-C9-N1-C2
3	A	501	NA7	O4D-C4D-C5D-O5D
3	C	501	NA7	O4D-C4D-C5D-O5D
3	C	501	NA7	C3D-C4D-C5D-O5D
3	A	501	NA7	C1B-C2B-O2B-P2B
3	D	501	NA7	C1B-C2B-O2B-P2B
3	B	501	NA7	C3B-C2B-O2B-P2B
5	B	1452	PEG	O1-C1-C2-O2
5	A	1455	PEG	O1-C1-C2-O2
5	B	1453	PEG	O2-C3-C4-O4
3	C	501	NA7	C1B-C2B-O2B-P2B
3	C	501	NA7	C3B-C2B-O2B-P2B
3	D	501	NA7	C3B-C2B-O2B-P2B
5	A	1454	PEG	O2-C3-C4-O4
5	B	1451	PEG	O2-C3-C4-O4
5	B	1452	PEG	O2-C3-C4-O4
4	D	1452	EPE	N4-C7-C8-O8
2	B	500	FAD	O4'-C4'-C5'-O5'
3	B	501	NA7	C3D-C4D-C5D-O5D
5	B	1451	PEG	O1-C1-C2-O2
2	B	500	FAD	C3'-C4'-C5'-O5'
4	D	1452	EPE	C9-C10-S-O3S
5	A	1455	PEG	O2-C3-C4-O4
5	B	1451	PEG	C4-C3-O2-C2
2	C	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	O3'-C3'-C4'-C5'
3	B	501	NA7	O4D-C4D-C5D-O5D
4	A	1452	EPE	C10-C9-N1-C6
4	A	1452	EPE	C8-C7-N4-C5
2	C	500	FAD	C2'-C3'-C4'-C5'
2	B	500	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
5	A	1453	PEG	C1-C2-O2-C3
3	D	501	NA7	C5B-O5B-PA-O3
3	C	501	NA7	C5D-O5D-PN-O1N
5	A	1454	PEG	C4-C3-O2-C2
4	D	1452	EPE	C9-C10-S-O1S
4	D	1452	EPE	C9-C10-S-O2S
4	D	1452	EPE	C8-C7-N4-C3
5	B	1452	PEG	C1-C2-O2-C3
5	A	1455	PEG	C4-C3-O2-C2
5	B	1453	PEG	C4-C3-O2-C2
2	C	500	FAD	O3'-C3'-C4'-O4'
2	B	500	FAD	C3B-C4B-C5B-O5B
5	B	1453	PEG	C1-C2-O2-C3
3	B	501	NA7	C1B-C2B-O2B-P2B
2	A	500	FAD	O4B-C4B-C5B-O5B
3	C	501	NA7	O4B-C4B-C5B-O5B
3	D	501	NA7	C3D-C4D-C5D-O5D
3	B	501	NA7	C5D-O5D-PN-O3
3	D	501	NA7	C5D-O5D-PN-O3
3	D	501	NA7	O4B-C4B-C5B-O5B
3	D	501	NA7	O4D-C4D-C5D-O5D
3	A	501	NA7	C5D-O5D-PN-O1N
3	C	501	NA7	C5B-O5B-PA-O1A
2	D	500	FAD	O4B-C4B-C5B-O5B
3	A	501	NA7	O4B-C4B-C5B-O5B
3	B	501	NA7	O4B-C4B-C5B-O5B
5	A	1453	PEG	O1-C1-C2-O2
5	A	1454	PEG	C1-C2-O2-C3
2	B	500	FAD	C2'-C1'-N10-C10

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NA7	2	0
2	A	500	FAD	2	0
3	B	501	NA7	4	0
5	A	1454	PEG	1	0
3	D	501	NA7	4	0
2	B	500	FAD	1	0
5	A	1453	PEG	5	0
3	C	501	NA7	2	0

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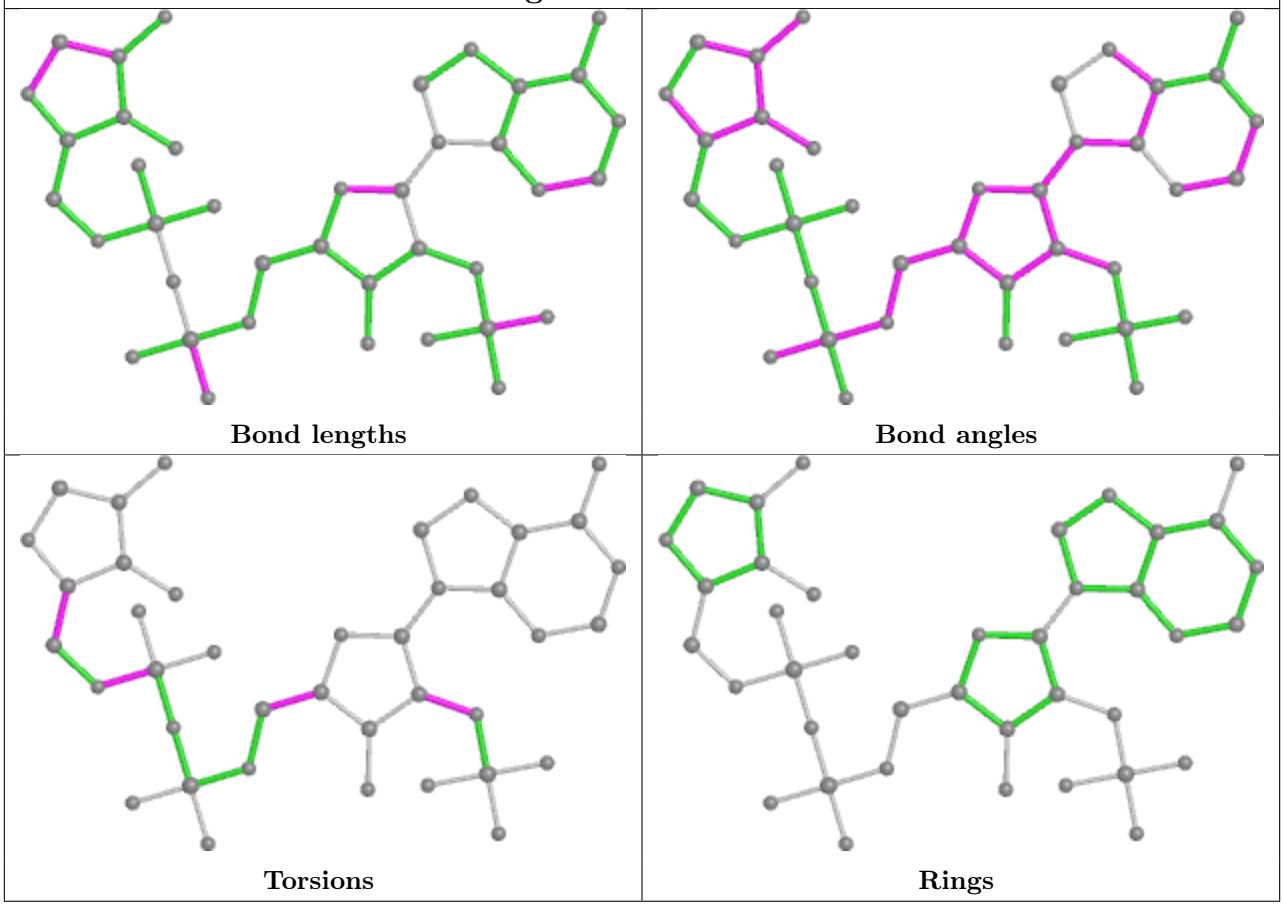
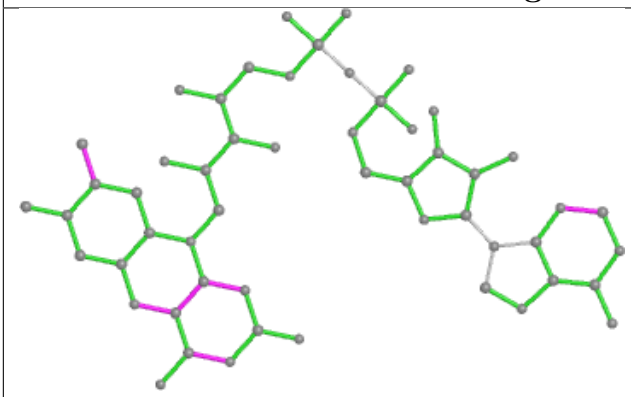
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1451	PEG	1	0
2	D	500	FAD	4	0
5	B	1452	PEG	1	0
2	C	500	FAD	3	0
4	A	1452	EPE	1	0

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.

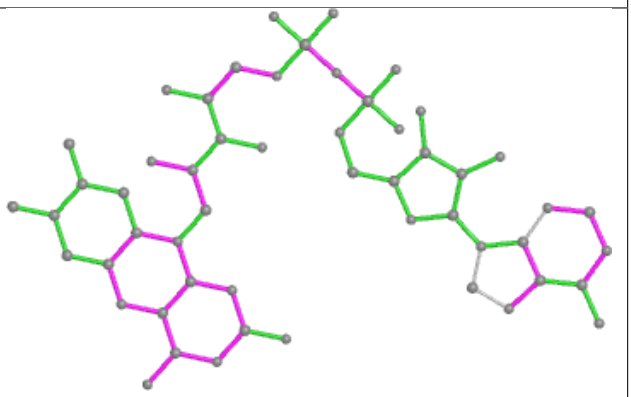
Ligand NA7 A 501



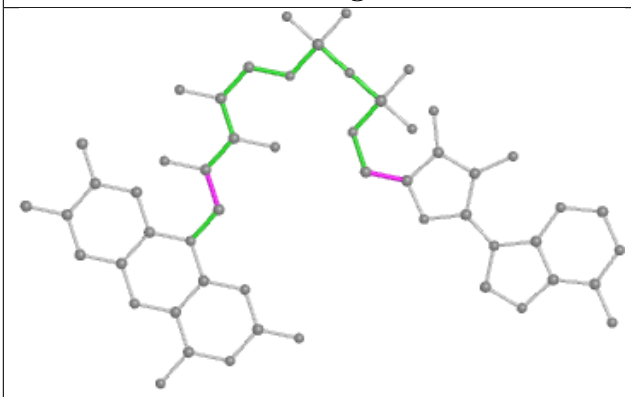
Ligand FAD A 500



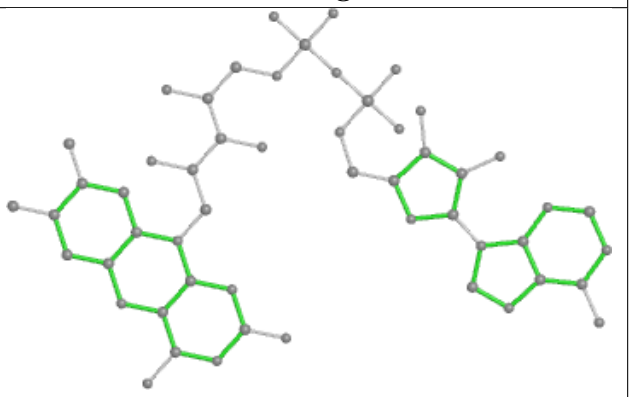
Bond lengths



Bond angles

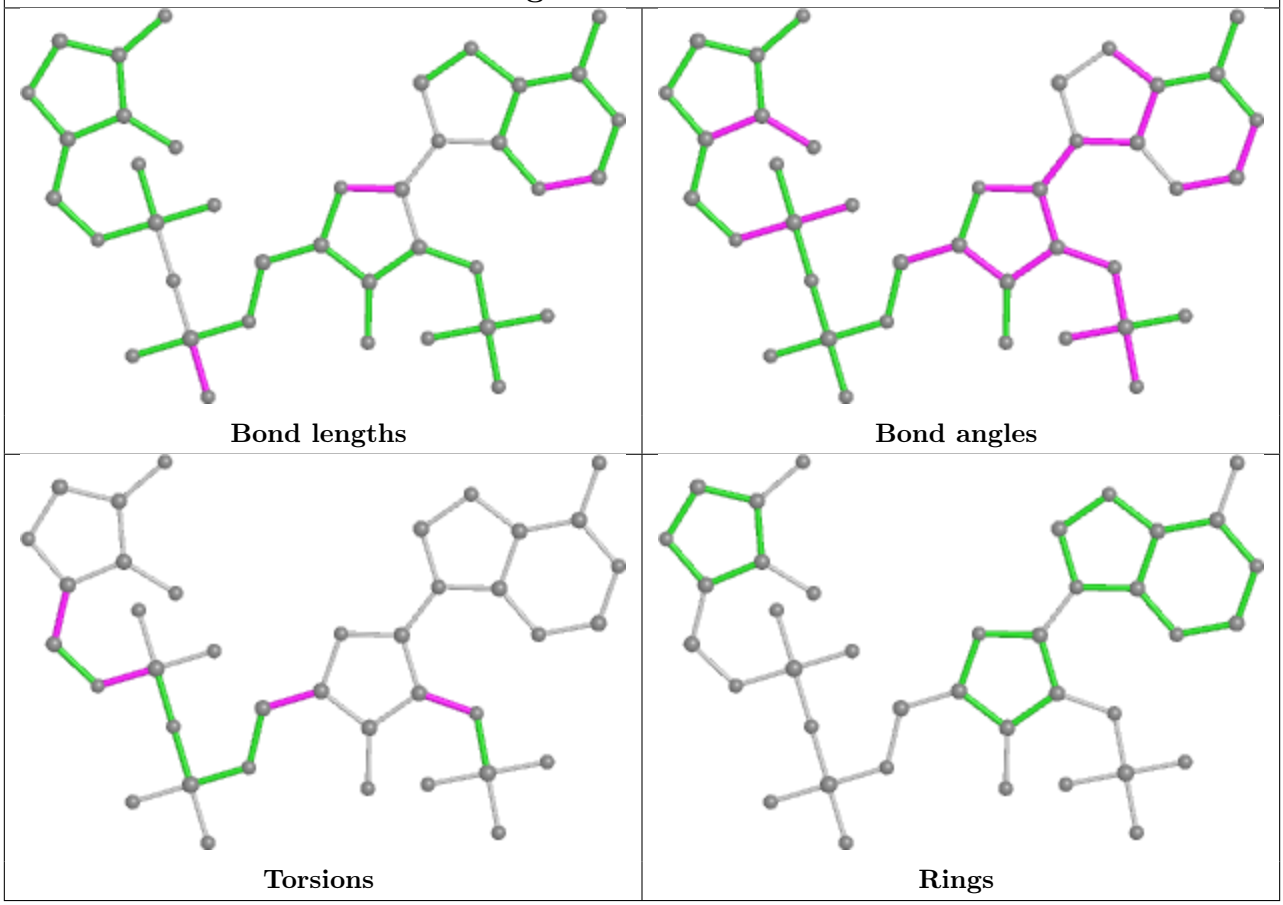


Torsions

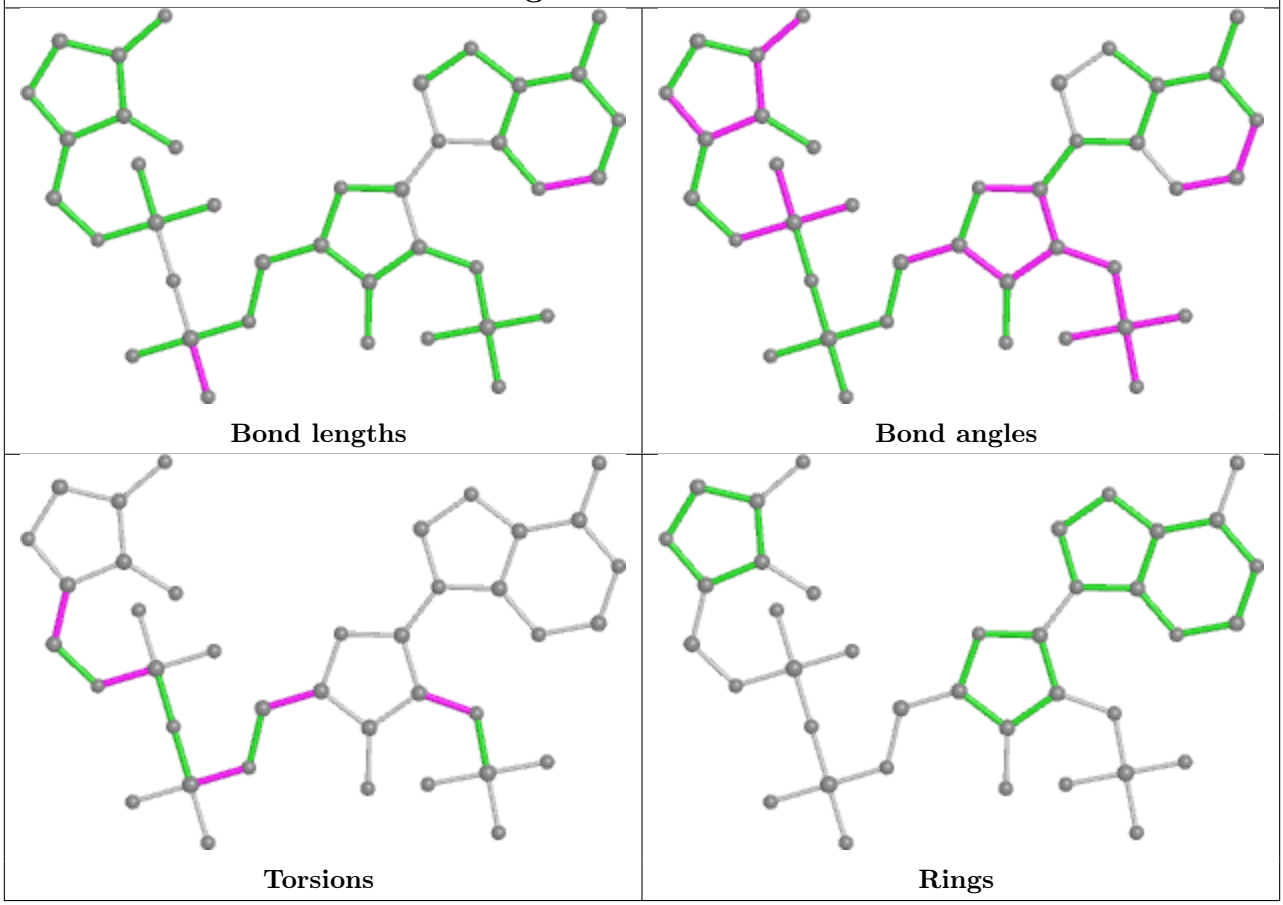


Rings

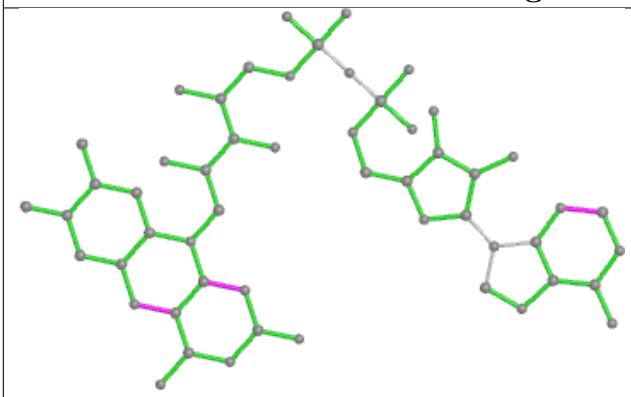
Ligand NA7 B 501



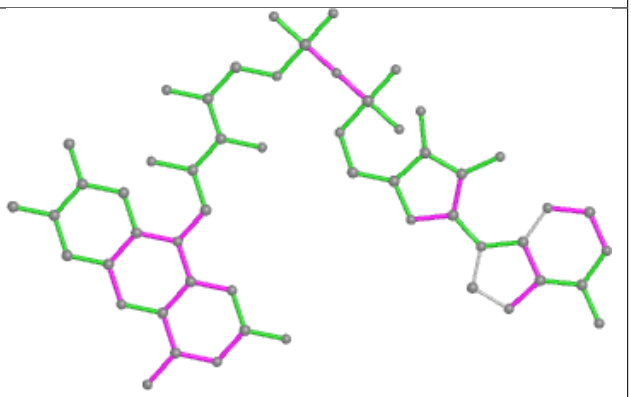
Ligand NA7 D 501



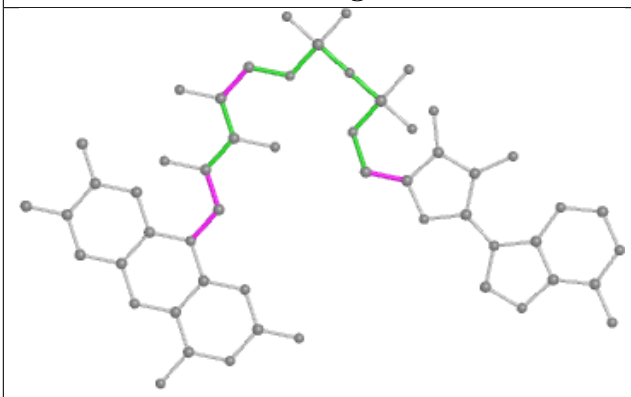
Ligand FAD B 500



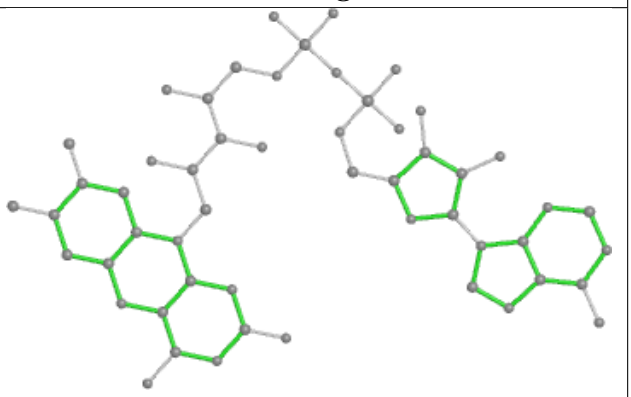
Bond lengths



Bond angles

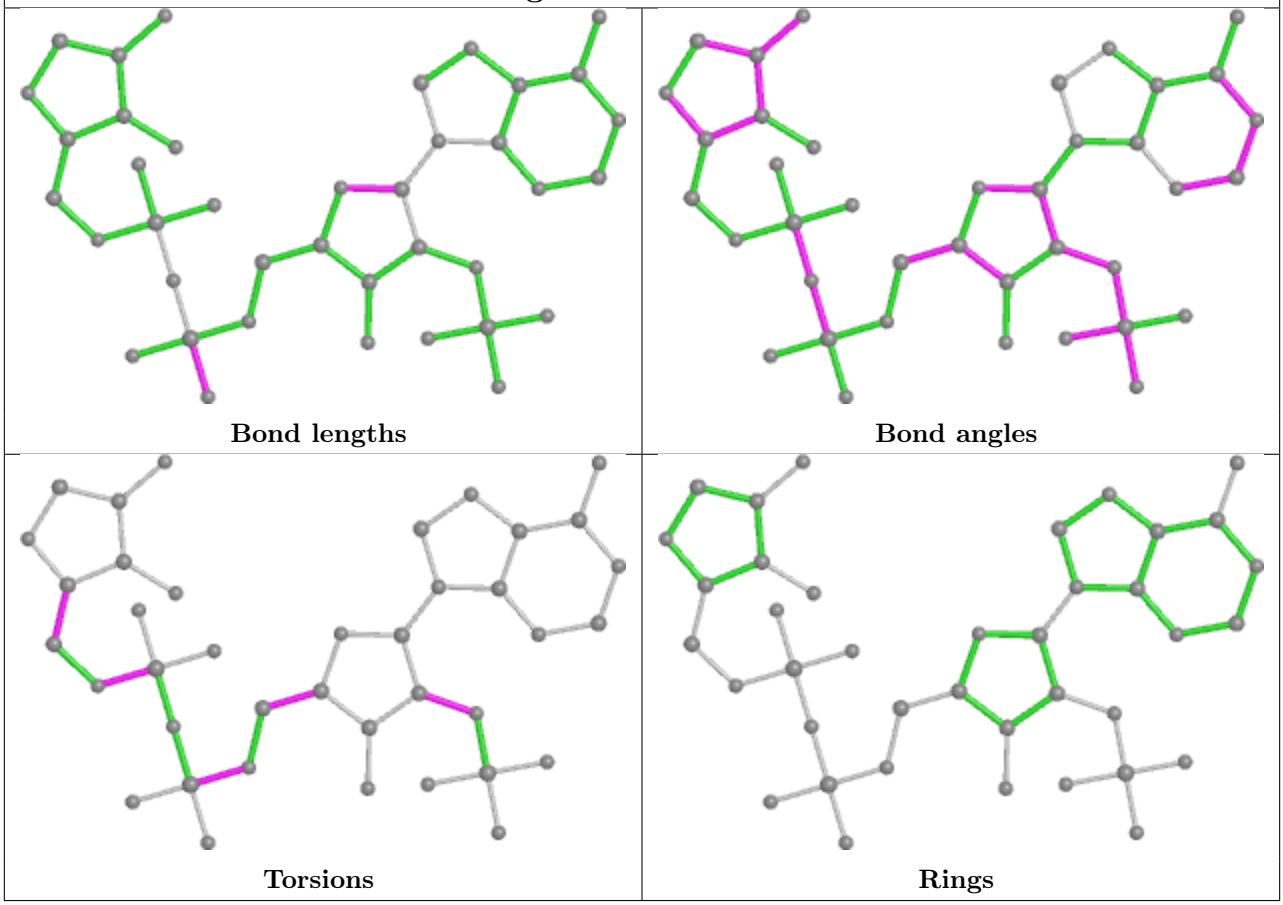


Torsions

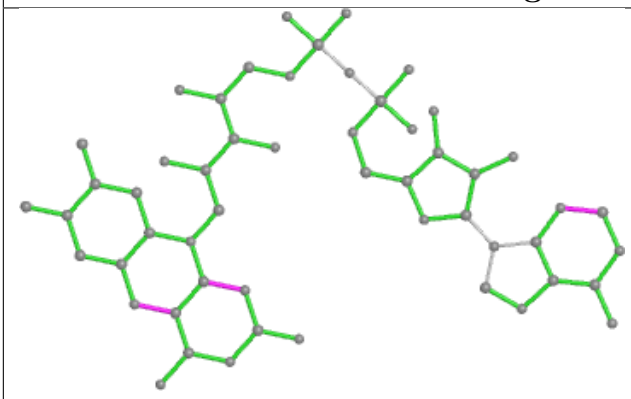


Rings

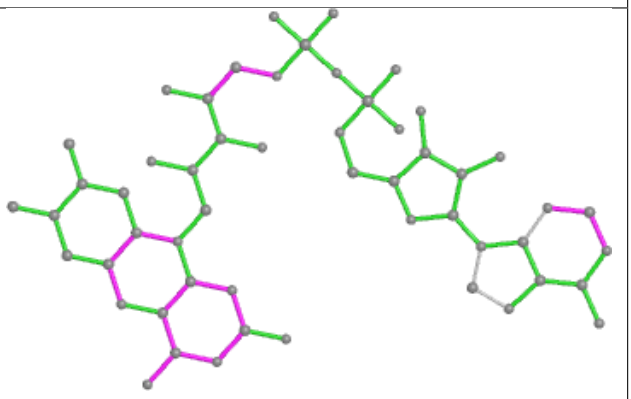
Ligand NA7 C 501



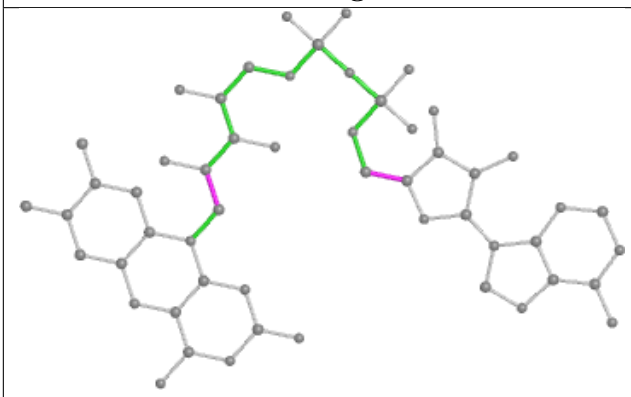
Ligand FAD D 500



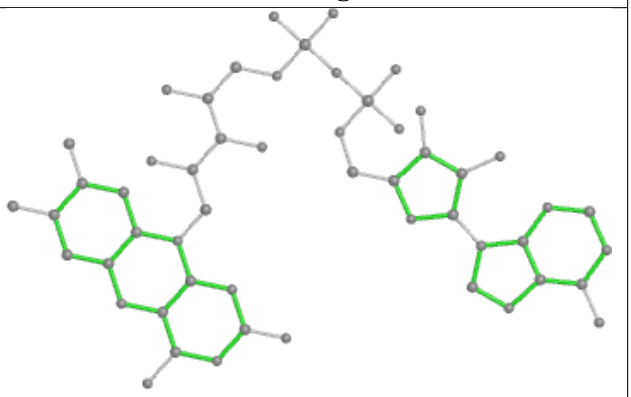
Bond lengths



Bond angles

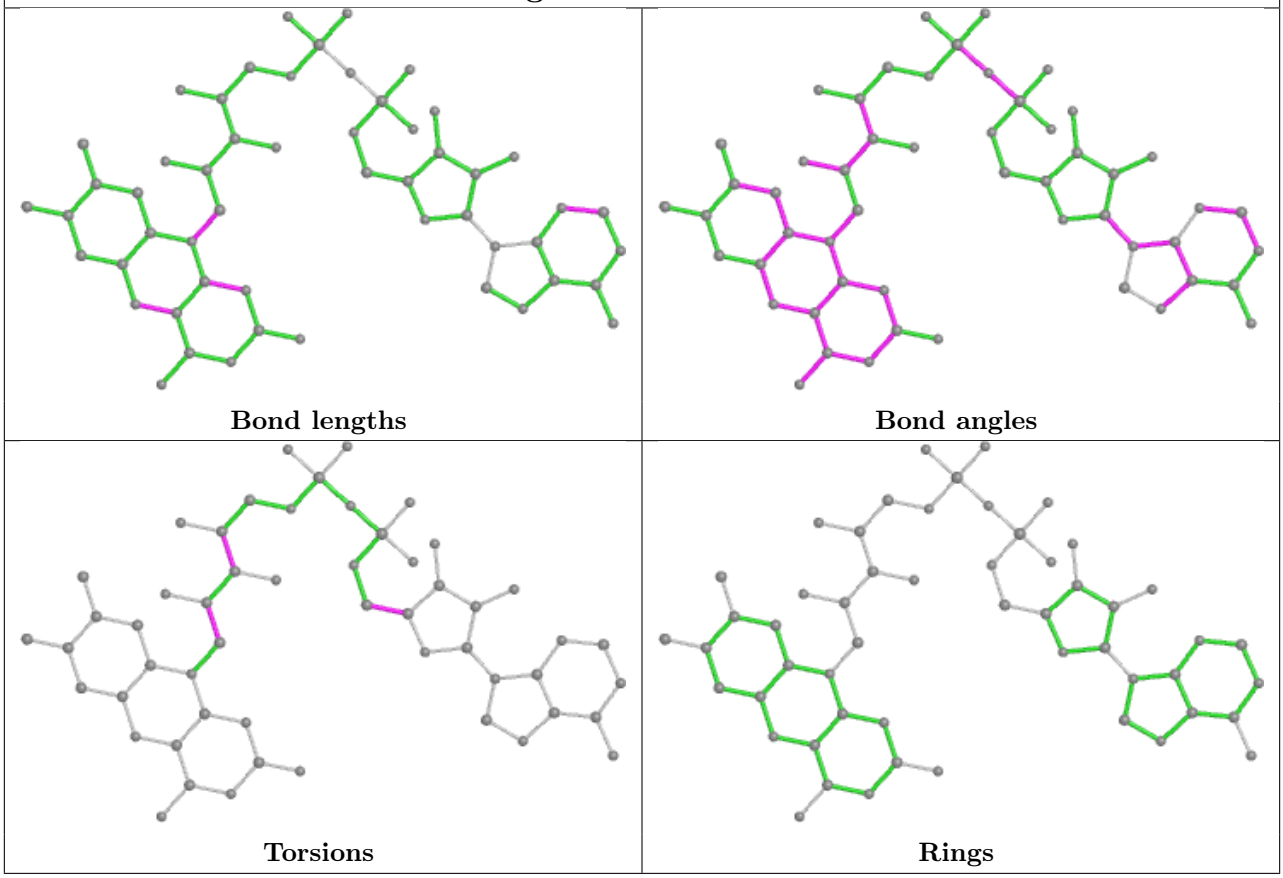


Torsions



Rings

Ligand FAD C 500



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	446/461 (96%)	-0.55	1 (0%)	95	95	16, 27, 42, 55	0
1	B	445/461 (96%)	-0.53	1 (0%)	95	95	15, 28, 43, 53	0
1	C	445/461 (96%)	-0.46	2 (0%)	92	91	16, 28, 44, 53	0
1	D	446/461 (96%)	-0.59	0	100	100	16, 27, 44, 52	0
All	All	1782/1844 (96%)	-0.53	4 (0%)	95	95	15, 27, 44, 55	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	ALA	2.5
1	C	423	SER	2.4
1	C	239	GLY	2.4
1	B	450	SER	2.1

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)

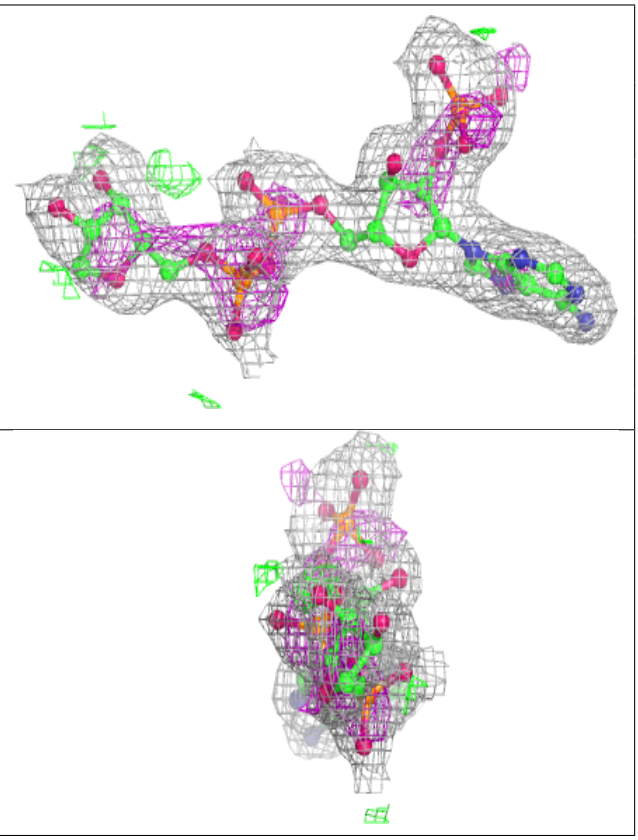
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	A	1453	7/7	0.85	0.23	33,36,42,47	0
5	PEG	B	1451	7/7	0.85	0.14	31,32,34,35	0
5	PEG	A	1454	7/7	0.86	0.22	33,38,46,46	0
4	EPE	D	1452	15/15	0.86	0.24	73,75,80,81	0
5	PEG	B	1452	7/7	0.86	0.20	33,40,42,42	0
5	PEG	B	1453	7/7	0.87	0.20	48,51,53,54	0
4	EPE	A	1452	15/15	0.88	0.22	68,71,78,78	0
5	PEG	A	1455	7/7	0.90	0.18	48,48,51,52	0
3	NA7	C	501	39/39	0.94	0.13	24,26,32,34	0
3	NA7	B	501	39/39	0.95	0.13	24,27,32,33	0
3	NA7	A	501	39/39	0.96	0.14	23,27,34,35	0
3	NA7	D	501	39/39	0.96	0.12	22,26,32,32	0
2	FAD	B	500	53/53	0.97	0.13	9,20,32,34	0
2	FAD	A	500	53/53	0.98	0.14	11,20,30,32	0
2	FAD	C	500	53/53	0.98	0.13	12,20,32,33	0
2	FAD	D	500	53/53	0.98	0.12	13,20,32,34	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.

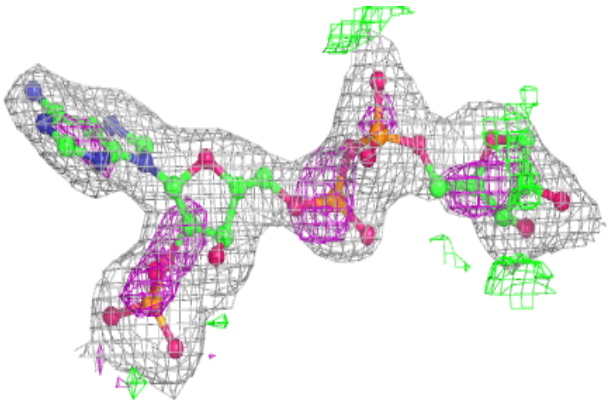
Electron density around NA7 C 501:

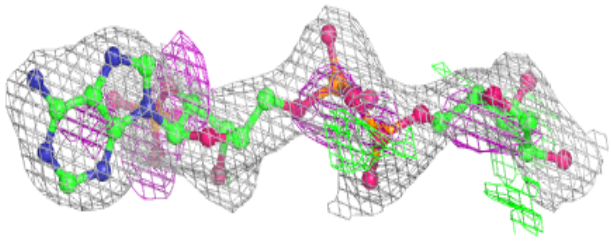
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

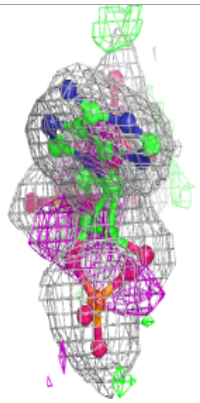


Electron density around NA7 B 501:

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

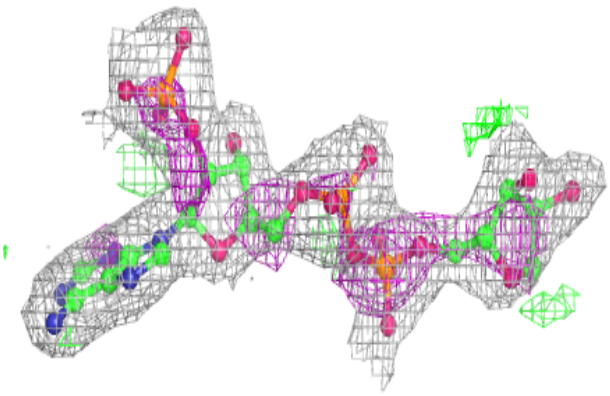


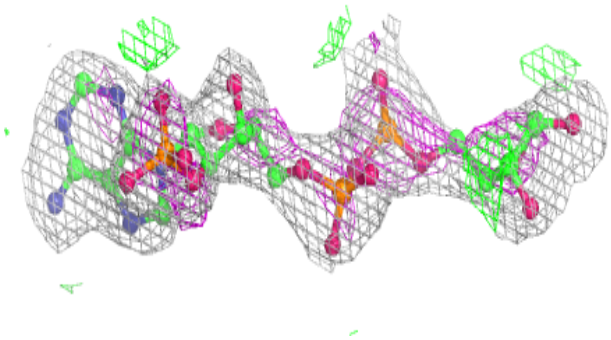


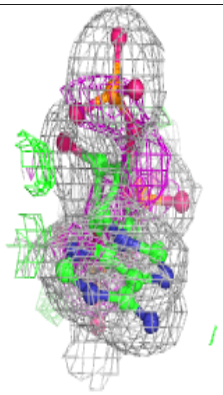


Electron density around NA7 A 501:

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

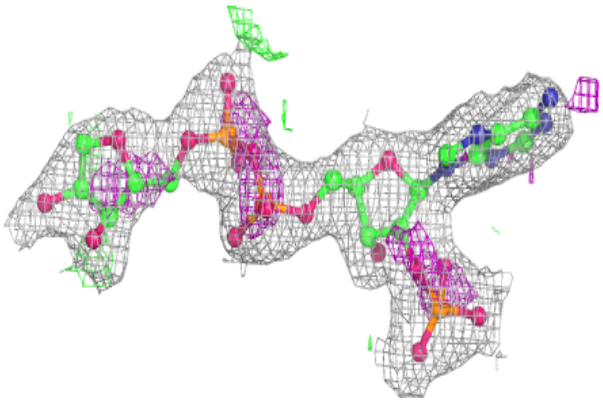


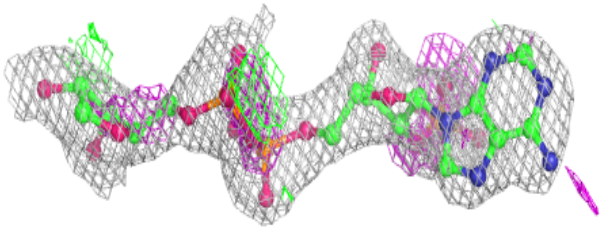


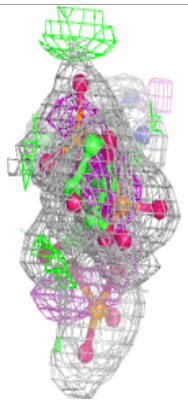


Electron density around NA7 D 501:

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

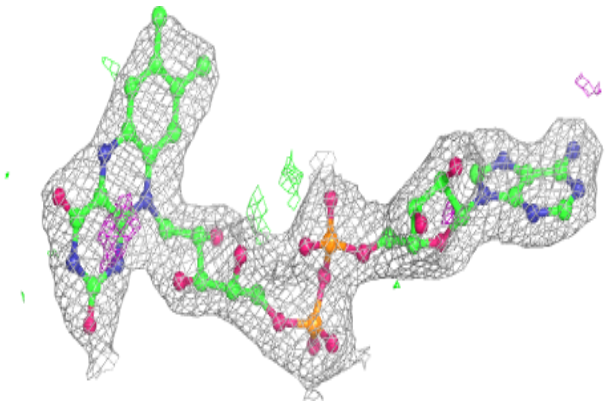


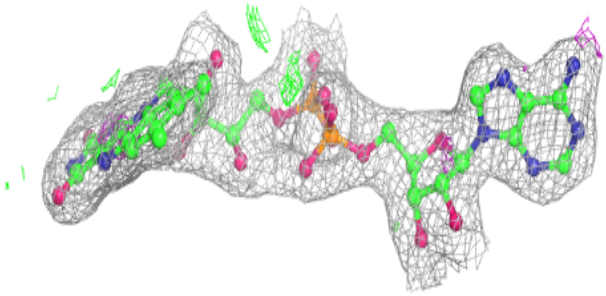


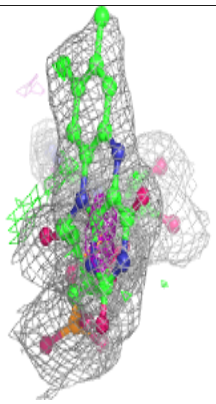


Electron density around FAD B 500:

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

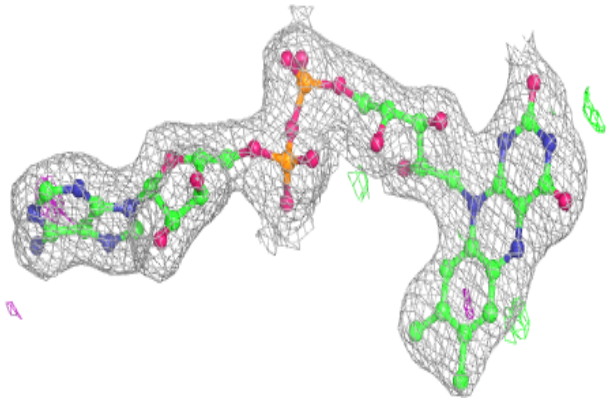


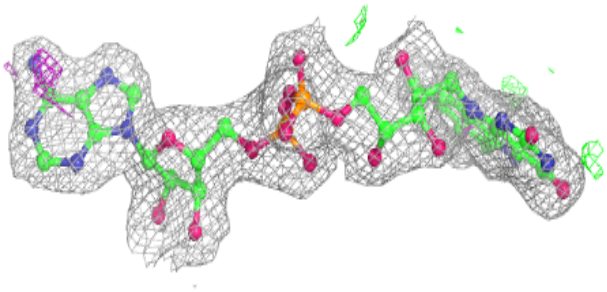


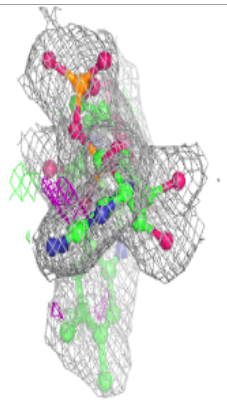


Electron density around FAD A 500:

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

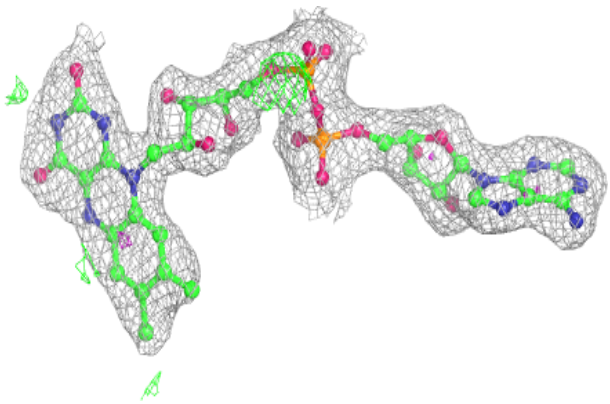


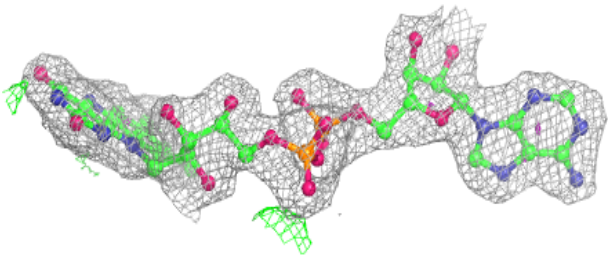


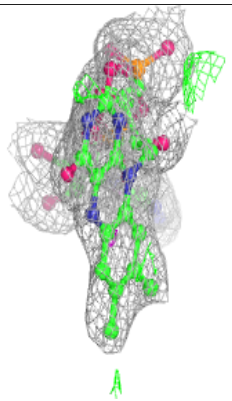


Electron density around FAD C 500:

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

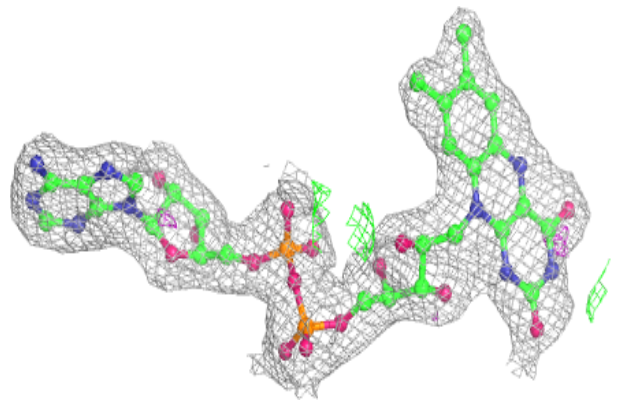


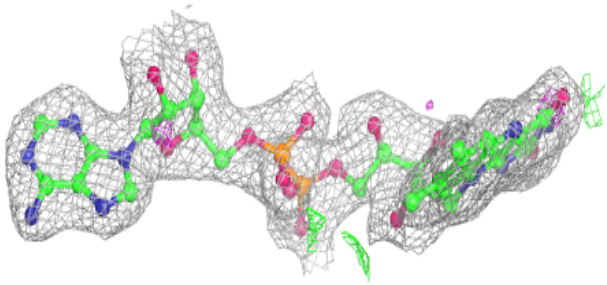


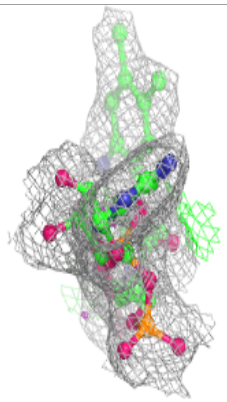


Electron density around FAD D 500:

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







6.5 Other polymers (i)

There are no such residues in this entry.