



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:24 AM UTC

PDB ID : 4TMC / pdb_00004tmc
Title : CRYSTAL STRUCTURE of OLD YELLOW ENZYME from CANDIDA MACEDONIENSIS AKU4588 COMPLEXED with P-HYDROXYBENZALDEHYDE
Authors : Horita, S.; Kataoka, M.; Kitamura, N.; Nakagawa, T.; Miyakawa, T.; Ohtsuka, J.; Nagata, K.; Shimizu, S.; Tanokura, M.
Deposited on : 2014-05-31
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

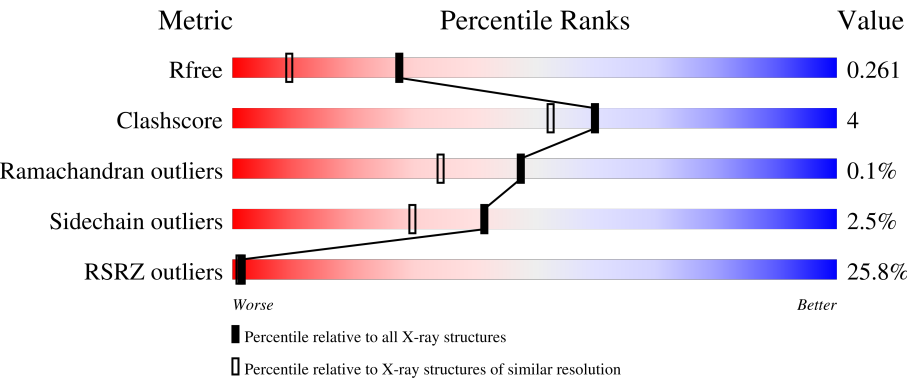
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

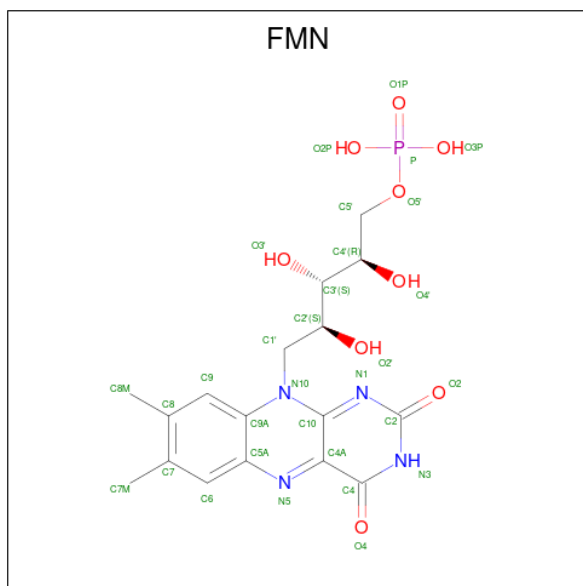
Mol	Chain	Length	Quality of chain
1	A	403	90%8%..
1	B	403	3% 88%10%..
1	C	403	89%8%..
1	D	403	98% 83%12%..

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 Old yellow enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total 3209	C 2055	N 543	O 605	S 6	0	0	0
1	B	398	Total 3200	C 2050	N 542	O 602	S 6	0	0	0
1	C	399	Total 3209	C 2055	N 543	O 605	S 6	0	0	0
1	D	396	Total 3182	C 2038	N 538	O 600	S 6	0	0	0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



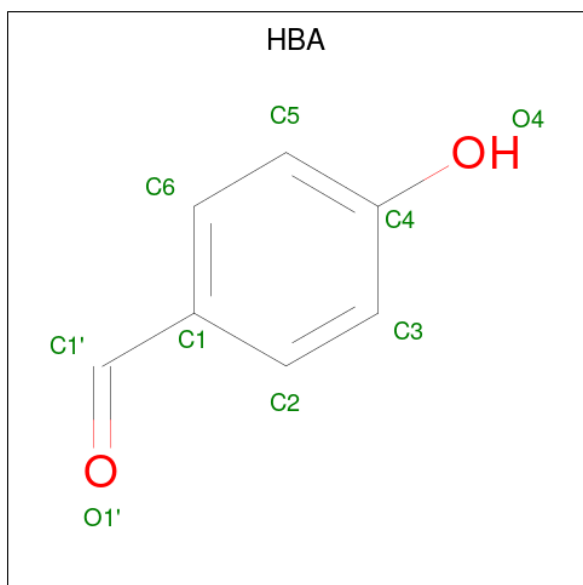
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is P-HYDROXYBENZALDEHYDE (CCD ID: HBA) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	7	2		
3	B	1	Total	C	O	0	0
			9	7	2		
3	C	1	Total	C	O	0	0
			9	7	2		
3	D	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		
4	B	254	Total	O	0	0
			254	254		
4	C	280	Total	O	0	0
			280	280		

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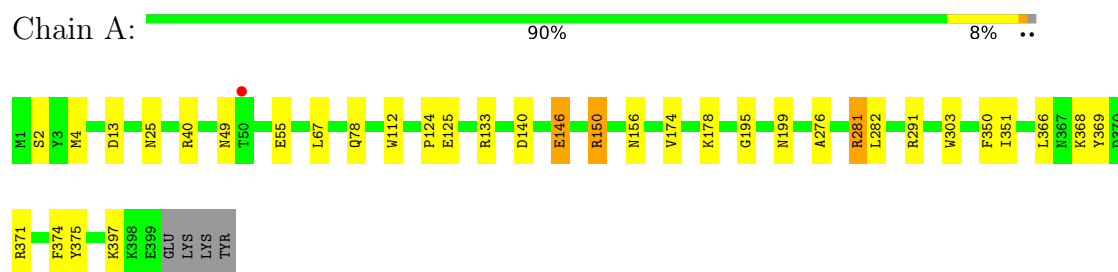
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	206	Total 206	O 206	0	0

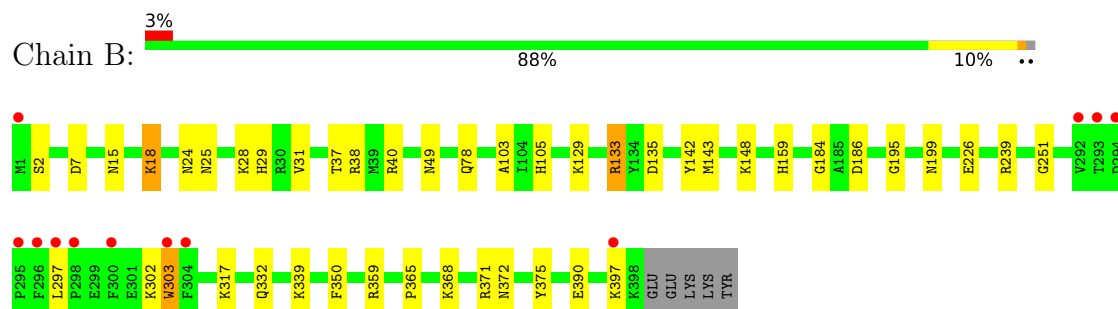
3 Residue-property plots

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.

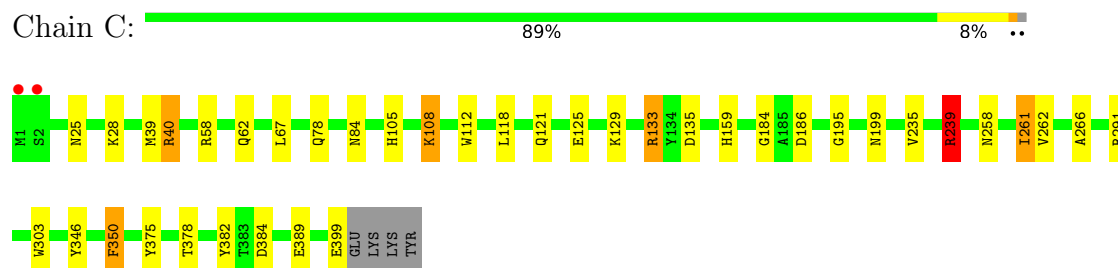
- Molecule 1: Old yellow enzyme



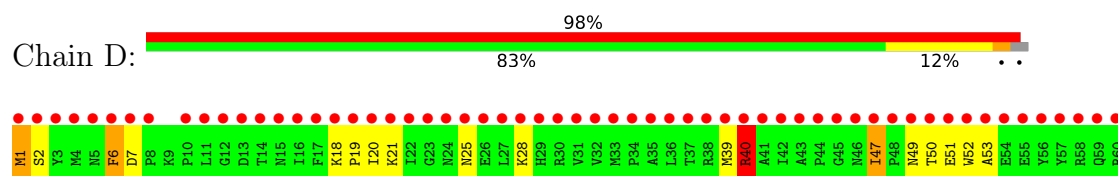
- Molecule 1: Old yellow enzyme



- Molecule 1: Old yellow enzyme



- Molecule 1: Old yellow enzyme



E361	Q62	S61	Q121	I181	S941	E301	E361
K362	A122	Q62	A122	D182	I242	K302	K362
G363	W123	Y63	W123	A183	R243	W303	G363
L364	P124	P64	P124	G184	F244	F304	L364
P365	E125	G65	E125	A185	S245	K305	P365
L366	A185	T66	A185	D186	P246	E306	L366
K367	V126	L67	V126	G187	Y247	G307	K367
K368	L127	L68	L127	V188	G248	T308	K368
Y369	K128	I68	K128	Q189	T249	N309	Y369
D370	K129	I69	K129	I190	F250	E310	D370
R371	G130	T70	G130	H191	G251	F311	R371
N372	G131	E71	N372	S192	T252	I312	N372
T373	G132	G72	T373	A193	M253	Y313	T373
F374	R133	T73	F374	H194	S254	S314	F374
T375	Y134	F74	T375	G195	G255	I315	T375
T376	D135	P75	T376	Y196	G256	W316	T376
F377	A137	S76	F377	L197	E257	K317	F377
T378	T138	Q77	T378	L198	N258	G318	T378
K379	D139	S79	K379	N199	P259	P319	K379
E380	D140	G80	E380	Q200	G260	V320	E380
G381	L141	G81	G381	F201	I261	L321	G381
Y382	Y142	Y82	Y382	L202	V262	R322	Y382
T383	M143	P83	T383	D203	A263	V323	T383
D384	G144	N84	D384	P204	Q264	G324	D384
Y385	E145	W85	Y385	I205	Y265	N325	Y385
P386	E146	P86	P386	S206	A266	Y326	P386
S387	E147	G87	S387	N207	Y267	A327	S387
Y388	K148	I88	Y388	M208	V268	L328	Y388
E389	E149	W89	E389	R209	I269	D329	E389
E390	R150	S90	E390	T210	G270	P330	E390
S391	A151	K91	S391	D211	E271	D331	S391
V392	L152	E92	V392	E212	L272	Q332	V392
A393	K153	Q93	A393	Y213	E273	A333	A393
K394	A154	L94	K394	G214	K274	T334	K394
G395	N155	A95	G395	G215	R275	L335	G395
Y396	N156	E96	Y396	S216	A276	D336	Y396
LYS	P157	W97	LYS	I217	R277	S337	LYS
LYS	Q158	K98	LYS	E218	A278	K338	LYS
GLU	H159	K99	GLU	N219	G279	K339	GLU
GLU	G160	I100	GLU	R220	K280	P340	GLU
LYS	I161	F101	LYS	A221	R281	N341	LYS
LYS	T162	N102	LYS	R222	L282	T342	LYS
TYR	K163	A103	TYR	F223	A283	L343	TYR
	E164	I104		L224	F284	I344	
	E165	H105		E225	I285	G345	
	K167	E106		V227	D286	Y346	
	Q168	N107		V228	L287	G347	
	Y169	K108		D229	V288	R348	
	I170	S109		A230	E289	S349	
	K171	F110		R290	P290	F350	
	E172	V111		V291	R291	I351	
	Y173	W112		V292	V292	A352	
	V174	Q114		D293	T293	N353	
	D175	L115		D294	P295	P354	
	A176	W116		F296	L296	D355	
	A177	W117		L297	L297	L356	
	K178	L118		P298	R298	V357	
	K179	G119		E299	R358	F358	
	A180	R120		F300	E300	L360	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.39Å 151.03Å 199.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 1.80 19.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.95-1.80) 99.7 (19.95-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.167 , 0.205 0.240 , 0.261	Depositor DCC
R_{free} test set	7395 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14010	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.20	0/3293	1.10	3/4463 (0.1%)
1	B	1.22	6/3284 (0.2%)	1.15	11/4451 (0.2%)
1	C	1.14	4/3293 (0.1%)	1.16	12/4463 (0.3%)
1	D	1.09	2/3266 (0.1%)	1.11	9/4429 (0.2%)
All	All	1.17	12/13136 (0.1%)	1.13	35/17806 (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	D	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	ARG	CD-NE	-7.63	1.35	1.46
1	B	239	ARG	CD-NE	-7.55	1.35	1.46
1	B	226	GLU	C-O	6.73	1.31	1.24
1	C	239	ARG	CD-NE	-6.28	1.37	1.46
1	D	40	ARG	CD-NE	-6.26	1.37	1.46
1	C	266	ALA	C-O	5.98	1.31	1.24
1	D	177	ALA	C-O	5.78	1.30	1.24
1	B	103	ALA	C-O	5.52	1.30	1.24
1	B	332	GLN	C-O	-5.49	1.17	1.24
1	B	372	ASN	C-O	-5.45	1.17	1.24
1	C	389	GLU	CD-OE1	5.41	1.35	1.25
1	C	384	ASP	N-CA	5.04	1.52	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	ARG	NE-CZ-NH2	-11.15	109.16	119.20
1	C	40	ARG	NE-CZ-NH1	10.93	132.43	121.50
1	B	133	ARG	NE-CZ-NH2	-10.32	109.91	119.20
1	D	40	ARG	NE-CZ-NH2	-9.01	111.10	119.20
1	C	40	ARG	CD-NE-CZ	8.56	136.38	124.40
1	C	40	ARG	CB-CG-CD	8.27	130.32	111.30
1	D	40	ARG	CD-NE-CZ	7.83	135.37	124.40
1	D	40	ARG	NE-CZ-NH1	7.71	129.21	121.50
1	A	150	ARG	NE-CZ-NH1	7.39	128.90	121.50
1	C	62	GLN	CB-CA-C	-7.36	97.01	110.63
1	C	133	ARG	NE-CZ-NH2	-6.90	112.99	119.20
1	B	133	ARG	CD-NE-CZ	6.89	134.05	124.40
1	B	28	LYS	CB-CA-C	6.86	121.58	109.65
1	B	133	ARG	CB-CG-CD	-6.61	96.10	111.30
1	A	150	ARG	NE-CZ-NH2	-6.37	113.46	119.20
1	C	62	GLN	CA-CB-CG	6.30	126.70	114.10
1	B	133	ARG	NE-CZ-NH1	6.22	127.72	121.50
1	D	133	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	C	399	GLU	N-CA-CB	-5.76	100.70	110.50
1	D	40	ARG	CG-CD-NE	-5.76	99.34	112.00
1	B	133	ARG	CA-CB-CG	5.73	125.56	114.10
1	D	174	VAL	N-CA-C	5.71	115.91	110.42
1	B	18	LYS	CA-C-N	-5.61	113.92	119.92
1	B	18	LYS	C-N-CA	-5.61	113.92	119.92
1	C	108	LYS	CD-CE-NZ	5.59	129.80	111.90
1	C	133	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	D	53	ALA	N-CA-C	5.37	117.21	111.36
1	C	239	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	B	390	GLU	CA-CB-CG	5.19	124.48	114.10
1	A	351	ILE	N-CA-C	-5.17	105.45	110.42
1	B	24	ASN	CB-CA-C	-5.14	99.86	109.72
1	B	303	TRP	CA-CB-CG	5.13	123.34	113.60
1	D	299	GLU	CA-CB-CG	5.12	124.35	114.10
1	C	58	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	D	133	ARG	CB-CG-CD	-5.02	99.76	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3209	0	3138	27	0
1	B	3200	0	3132	26	0
1	C	3209	0	3138	24	0
1	D	3182	0	3106	34	0
2	A	31	0	19	1	0
2	B	31	0	19	1	0
2	C	31	0	19	0	0
2	D	31	0	19	2	0
3	A	9	0	5	0	0
3	B	9	0	5	0	0
3	C	9	0	5	0	0
3	D	9	0	5	0	0
4	A	310	0	0	1	0
4	B	254	0	0	3	0
4	C	280	0	0	1	0
4	D	206	0	0	5	0
All	All	14010	0	12610	110	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 4.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:MET:HE3	1:A:366:LEU:HB2	1.30	1.12
1:B:368:LYS:HG3	4:B:823:HOH:O	1.52	1.07
1:D:371:ARG:NH2	4:D:641:HOH:O	2.01	0.93
1:A:55:GLU:HG2	4:A:673:HOH:O	1.75	0.87
1:A:4:MET:CE	1:A:366:LEU:HB2	2.06	0.85
1:A:4:MET:HE3	1:A:366:LEU:CB	2.05	0.84
1:B:133:ARG:HD2	1:B:135:ASP:OD1	1.80	0.82
1:A:4:MET:CE	1:A:366:LEU:CB	2.58	0.81
1:C:78:GLN:HE22	1:C:133:ARG:H	1.31	0.79
1:A:78:GLN:HE22	1:A:133:ARG:H	1.32	0.77
1:A:146:GLU:H	1:A:146:GLU:CD	1.92	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:GLN:HE22	1:D:133:ARG:H	1.33	0.76
1:C:39:MET:HE2	1:C:375:TYR:HB3	1.68	0.75
1:B:195:GLY:H	1:B:199:ASN:HD22	1.36	0.74
1:A:124:PRO:HD2	1:A:150:ARG:HD2	1.70	0.73
1:A:125:GLU:OE1	1:A:150:ARG:HD3	1.88	0.73
1:D:195:GLY:H	1:D:199:ASN:HD22	1.38	0.72
1:C:67:LEU:HD11	1:C:112:TRP:CD1	2.27	0.69
1:B:29:HIS:HD2	1:B:31:VAL:H	1.40	0.68
1:C:40:ARG:HD3	1:C:378:THR:O	1.95	0.67
1:C:25:ASN:HD21	1:C:186:ASP:HB3	1.58	0.66
1:D:18:LYS:HG3	1:D:19:PRO:HD2	1.78	0.66
1:C:195:GLY:H	1:C:199:ASN:HD22	1.44	0.66
1:C:108:LYS:HE3	4:C:759:HOH:O	1.96	0.65
1:D:175:ASP:OD2	1:D:179:LYS:HE2	1.97	0.64
1:C:235:VAL:O	1:C:239:ARG:HD3	1.96	0.64
1:C:133:ARG:HD2	1:C:135:ASP:OD1	1.98	0.64
1:D:49:ASN:OD1	1:D:51:GLU:HG3	1.97	0.64
1:D:102:ASN:HB3	4:D:744:HOH:O	1.97	0.64
1:A:195:GLY:H	1:A:199:ASN:HD22	1.44	0.64
1:B:40:ARG:O	1:B:49:ASN:HB2	1.98	0.64
1:B:2:SER:HB2	1:B:397:LYS:O	1.99	0.62
1:C:235:VAL:O	1:C:239:ARG:CD	2.49	0.61
1:B:78:GLN:HE22	1:B:133:ARG:H	1.48	0.61
1:D:195:GLY:H	1:D:199:ASN:ND2	1.99	0.60
1:A:4:MET:CE	1:A:366:LEU:HB3	2.31	0.60
1:B:15:ASN:HD22	1:B:18:LYS:HD2	1.67	0.60
1:B:148:LYS:HE2	4:B:604:HOH:O	2.02	0.60
1:D:299:GLU:OE1	1:D:369:TYR:OH	2.15	0.59
1:B:375:TYR:CE1	2:B:501:FMN:HM71	2.39	0.58
1:C:258:ASN:HB3	1:C:261:ILE:HD13	1.87	0.56
1:C:195:GLY:H	1:C:199:ASN:ND2	2.03	0.56
1:D:133:ARG:HD2	1:D:135:ASP:OD1	2.06	0.56
1:D:348:ARG:HD3	2:D:501:FMN:O1P	2.05	0.56
1:D:280:LYS:CE	4:D:696:HOH:O	2.54	0.56
1:A:40:ARG:O	1:A:49:ASN:HB2	2.06	0.55
1:D:323:VAL:HG22	1:D:345:GLY:HA3	1.88	0.55
1:D:50:THR:OG1	1:D:96:GLU:HB3	2.06	0.55
1:D:40:ARG:O	1:D:49:ASN:HB2	2.07	0.55
1:B:148:LYS:CE	4:B:604:HOH:O	2.56	0.54
1:D:52:TRP:CE2	1:D:379:LYS:HG2	2.43	0.54
1:B:29:HIS:CD2	1:B:31:VAL:H	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:TYR:CE1	2:A:501:FMN:HM71	2.42	0.53
1:A:276:ALA:HB1	1:A:281:ARG:HB2	1.90	0.52
1:B:133:ARG:CD	1:B:135:ASP:OD1	2.56	0.51
1:B:317:LYS:HE2	1:D:306:GLU:HB3	1.92	0.51
1:D:102:ASN:CB	4:D:744:HOH:O	2.54	0.51
1:A:371:ARG:HD2	1:A:374:PHE:CD2	2.46	0.51
1:A:125:GLU:CD	1:A:150:ARG:HD3	2.36	0.51
1:D:1:MET:HE1	1:D:370:ASP:HB2	1.92	0.50
1:B:195:GLY:H	1:B:199:ASN:ND2	2.06	0.49
1:B:105:HIS:HE1	1:B:184:GLY:O	1.95	0.49
1:A:276:ALA:CB	1:A:281:ARG:HB2	2.43	0.49
1:A:4:MET:HE1	1:A:366:LEU:CD1	2.43	0.48
1:D:50:THR:HG21	1:D:99:LYS:HD3	1.95	0.48
1:C:261:ILE:HG22	1:C:262:VAL:N	2.27	0.48
1:D:280:LYS:HE2	4:D:696:HOH:O	2.11	0.48
1:C:40:ARG:HD2	1:C:382:TYR:CD1	2.49	0.48
1:D:67:LEU:HD11	1:D:112:TRP:CD1	2.48	0.48
1:B:297:LEU:HD13	1:B:302:LYS:HG2	1.96	0.47
1:A:140:ASP:OD1	1:A:140:ASP:N	2.47	0.47
1:B:297:LEU:HD13	1:B:302:LYS:CG	2.45	0.46
1:D:296:PHE:HA	1:D:371:ARG:NH2	2.30	0.46
1:C:39:MET:CE	1:C:375:TYR:HB3	2.43	0.46
1:D:20:ILE:CD1	1:D:341:ASN:HD22	2.28	0.46
1:A:25:ASN:ND2	1:A:112:TRP:HE1	2.13	0.46
1:A:291:ARG:HA	1:A:303:TRP:CD1	2.51	0.46
1:B:15:ASN:ND2	1:B:18:LYS:HD2	2.31	0.46
1:C:133:ARG:HD3	1:C:159:HIS:CD2	2.52	0.45
1:C:67:LEU:CD1	1:C:112:TRP:CD1	2.98	0.45
1:A:2:SER:HB2	1:A:397:LYS:O	2.17	0.45
1:A:195:GLY:H	1:A:199:ASN:ND2	2.12	0.45
1:C:125:GLU:O	1:C:129:LYS:HD3	2.17	0.44
1:C:235:VAL:O	1:C:239:ARG:HD2	2.18	0.44
1:D:387:SER:OG	1:D:390:GLU:HG3	2.18	0.44
1:C:105:HIS:HE1	1:C:184:GLY:O	2.01	0.43
1:C:291:ARG:HA	1:C:303:TRP:CD1	2.53	0.43
1:D:47:ILE:HD12	1:D:92:GLU:HB3	2.00	0.43
1:D:348:ARG:CD	2:D:501:FMN:O1P	2.67	0.43
1:B:15:ASN:HA	1:B:18:LYS:HG3	2.00	0.43
1:B:133:ARG:HD3	1:B:159:HIS:CD2	2.53	0.43
1:A:368:LYS:HD2	1:A:369:TYR:H	1.84	0.43
1:C:39:MET:HA	1:C:84:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:PHE:CG	1:D:7:ASP:N	2.87	0.43
1:D:305:LYS:HE2	1:D:305:LYS:HB2	1.88	0.42
1:B:25:ASN:HD21	1:B:186:ASP:HB3	1.84	0.42
1:A:67:LEU:HD11	1:A:112:TRP:CD1	2.55	0.42
1:C:40:ARG:HD2	1:C:382:TYR:CG	2.55	0.42
1:B:142:TYR:CE2	1:B:148:LYS:HA	2.55	0.41
1:B:37:THR:O	1:B:38:ARG:HD2	2.20	0.41
1:D:39:MET:HA	1:D:84:ASN:O	2.20	0.41
1:A:174:VAL:CG1	1:A:178:LYS:HE3	2.51	0.41
1:B:359:ARG:HD3	1:B:365:PRO:O	2.21	0.41
1:D:28:LYS:HG3	1:D:65:GLY:HA3	2.02	0.41
1:B:143:MET:HE3	1:B:251:GLY:HA2	2.01	0.41
1:C:346:TYR:O	1:C:350:PHE:HB2	2.21	0.41
1:D:25:ASN:HD21	1:D:186:ASP:HB3	1.86	0.41
1:D:156:ASN:HD22	1:D:156:ASN:HA	1.72	0.41
1:D:346:TYR:HB3	1:D:349:SER:OG	2.21	0.40
1:A:146:GLU:CD	1:A:146:GLU:N	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	397/403 (98%)	386 (97%)	11 (3%)	0	100	100
1	B	396/403 (98%)	382 (96%)	14 (4%)	0	100	100
1	C	397/403 (98%)	385 (97%)	12 (3%)	0	100	100
1	D	394/403 (98%)	379 (96%)	14 (4%)	1 (0%)	36	25
All	All	1584/1612 (98%)	1532 (97%)	51 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	6	PHE

5.3.2 Protein sidechains ⓘ

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	336/340 (99%)	330 (98%)	6 (2%)	51	43
1	B	335/340 (98%)	329 (98%)	6 (2%)	51	43
1	C	336/340 (99%)	330 (98%)	6 (2%)	51	43
1	D	333/340 (98%)	318 (96%)	15 (4%)	24	12
All	All	1340/1360 (98%)	1307 (98%)	33 (2%)	42	30

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	146	GLU
1	A	156	ASN
1	A	281	ARG
1	A	282	LEU
1	A	350	PHE
1	B	7	ASP
1	B	129	LYS
1	B	303	TRP
1	B	339	LYS
1	B	350	PHE
1	B	371	ARG
1	C	28	LYS
1	C	118	LEU
1	C	121	GLN
1	C	239	ARG
1	C	261	ILE
1	C	350	PHE
1	D	2	SER
1	D	21	LYS
1	D	40	ARG

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Mol	Chain	Res	Type
1	D	47	ILE
1	D	91	LYS
1	D	141	LEU
1	D	146	GLU
1	D	156	ASN
1	D	261	ILE
1	D	299	GLU
1	D	305	LYS
1	D	348	ARG
1	D	350	PHE
1	D	379	LYS
1	D	396	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	78	GLN
1	A	107	ASN
1	A	156	ASN
1	A	158	GLN
1	A	199	ASN
1	B	5	ASN
1	B	15	ASN
1	B	25	ASN
1	B	29	HIS
1	B	78	GLN
1	B	102	ASN
1	B	199	ASN
1	C	25	ASN
1	C	78	GLN
1	C	102	ASN
1	C	121	GLN
1	C	155	ASN
1	C	199	ASN
1	C	372	ASN
1	D	15	ASN
1	D	25	ASN
1	D	78	GLN
1	D	156	ASN
1	D	168	GLN
1	D	199	ASN

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Mol	Chain	Res	Type
1	D	332	GLN
1	D	341	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FMN	B	501	-	33,33,33	1.90	8 (24%)	48,50,50	1.66	12 (25%)
2	FMN	D	501	-	33,33,33	1.66	7 (21%)	48,50,50	1.36	9 (18%)
2	FMN	C	501	-	33,33,33	1.20	4 (12%)	48,50,50	1.54	9 (18%)
3	HBA	B	502	-	9,9,9	1.00	0	11,11,11	1.04	0
3	HBA	A	502	-	9,9,9	0.70	0	11,11,11	1.40	1 (9%)
3	HBA	C	502	-	9,9,9	1.00	0	11,11,11	1.02	0
3	HBA	D	502	-	9,9,9	0.88	0	11,11,11	1.10	1 (9%)
2	FMN	A	501	-	33,33,33	1.74	7 (21%)	48,50,50	1.60	11 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	501	-	-	1/18/18/18	0/3/3/3
2	FMN	D	501	-	-	1/18/18/18	0/3/3/3
2	FMN	C	501	-	-	2/18/18/18	0/3/3/3
3	HBA	B	502	-	-	0/2/2/2	0/1/1/1
3	HBA	A	502	-	-	0/2/2/2	0/1/1/1
3	HBA	C	502	-	-	0/2/2/2	0/1/1/1
3	HBA	D	502	-	-	0/2/2/2	0/1/1/1
2	FMN	A	501	-	-	1/18/18/18	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FMN	C9A-C5A	5.51	1.50	1.41
2	B	501	FMN	C1'-C2'	4.90	1.59	1.52
2	A	501	FMN	C5'-C4'	4.55	1.58	1.51
2	B	501	FMN	C8-C7	3.67	1.49	1.40
2	D	501	FMN	C9A-C5A	3.60	1.47	1.41
2	A	501	FMN	C4A-N5	3.50	1.38	1.30
2	D	501	FMN	O4-C4	3.30	1.29	1.23
2	D	501	FMN	C5'-C4'	3.17	1.56	1.51
2	A	501	FMN	C9A-C5A	3.07	1.46	1.41
2	B	501	FMN	C5'-C4'	3.07	1.56	1.51
2	A	501	FMN	O3'-C3'	2.87	1.50	1.43
2	D	501	FMN	O2-C2	2.81	1.29	1.24
2	D	501	FMN	P-O5'	2.54	1.68	1.60
2	D	501	FMN	C10-N1	2.54	1.38	1.33
2	C	501	FMN	O4-C4	2.47	1.28	1.23
2	B	501	FMN	O4-C4	2.40	1.28	1.23
2	D	501	FMN	C8-C7	2.32	1.46	1.40
2	B	501	FMN	C4A-N5	2.29	1.35	1.30
2	C	501	FMN	C5A-N5	-2.26	1.35	1.39
2	B	501	FMN	C5A-N5	-2.22	1.35	1.39
2	A	501	FMN	O2'-C2'	2.20	1.47	1.43
2	A	501	FMN	C1'-C2'	2.19	1.55	1.52
2	B	501	FMN	O3'-C3'	2.19	1.48	1.43
2	A	501	FMN	C4A-C10	2.12	1.50	1.44
2	C	501	FMN	C2-N3	-2.02	1.34	1.39
2	C	501	FMN	C8M-C8	-2.00	1.47	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FMN	O2-C2-N1	-5.19	113.18	121.80
2	A	501	FMN	C9A-C5A-N5	-3.76	118.46	122.45
2	C	501	FMN	C7M-C7-C6	3.63	125.96	119.57
2	A	501	FMN	C4-C4A-N5	3.55	123.12	118.21
2	B	501	FMN	C4-C4A-N5	3.49	123.03	118.21
2	C	501	FMN	C4-C4A-N5	3.47	123.00	118.21
2	A	501	FMN	C5A-C9A-N10	3.37	121.02	117.97
3	A	502	HBA	O1'-C1'-C1	-3.29	113.40	124.56
2	A	501	FMN	O2-C2-N1	-3.25	116.40	121.80
2	A	501	FMN	O3'-C3'-C4'	3.24	116.28	108.93
2	C	501	FMN	C5A-N5-C4A	3.10	123.11	118.09
2	A	501	FMN	O4-C4-C4A	-2.91	118.85	126.53
2	A	501	FMN	C5A-N5-C4A	2.83	122.66	118.09
2	D	501	FMN	C4-C4A-N5	2.78	122.05	118.21
2	D	501	FMN	O3P-P-O2P	2.71	117.97	107.80
2	B	501	FMN	O4-C4-C4A	-2.70	119.40	126.53
2	C	501	FMN	C10-C4A-N5	-2.70	119.30	124.81
2	B	501	FMN	C10-C4A-N5	-2.68	119.33	124.81
2	D	501	FMN	C4A-C10-N10	2.68	120.32	116.48
2	C	501	FMN	C7M-C7-C8	-2.58	115.49	120.76
2	B	501	FMN	C4A-C10-N10	2.57	120.16	116.48
2	D	501	FMN	O5'-P-O1P	-2.55	99.54	106.44
3	D	502	HBA	O1'-C1'-C1	-2.51	116.07	124.56
2	B	501	FMN	C4A-C10-N1	-2.47	118.53	124.59
2	D	501	FMN	C9A-N10-C10	-2.34	117.18	120.75
2	B	501	FMN	C4-N3-C2	-2.28	121.59	125.64
2	C	501	FMN	O2P-P-O5'	-2.28	100.72	106.67
2	A	501	FMN	O2'-C2'-C1'	2.27	119.52	110.20
2	A	501	FMN	C10-C4A-N5	-2.27	120.18	124.81
2	B	501	FMN	O2-C2-N3	2.26	122.92	118.58
2	D	501	FMN	C5A-C9A-N10	2.24	120.00	117.97
2	A	501	FMN	O4'-C4'-C3'	2.23	114.47	109.25
2	B	501	FMN	O3P-P-O1P	2.19	119.38	110.83
2	D	501	FMN	O2-C2-N1	-2.19	118.16	121.80
2	C	501	FMN	C9A-C5A-N5	-2.18	120.14	122.45
2	A	501	FMN	N3-C2-N1	2.18	124.14	119.50
2	C	501	FMN	O3P-P-O2P	2.16	115.90	107.80
2	D	501	FMN	O4-C4-C4A	-2.14	120.89	126.53
2	B	501	FMN	C10-N1-C2	2.12	121.44	116.85
2	D	501	FMN	O2P-P-O5'	-2.12	101.14	106.67
2	B	501	FMN	C5A-N5-C4A	2.07	121.44	118.09
2	B	501	FMN	N3-C2-N1	2.05	123.86	119.50
2	C	501	FMN	C4A-C10-N1	-2.04	119.58	124.59

There are no chirality outliers.

All (5) torsion outliers are listed below:

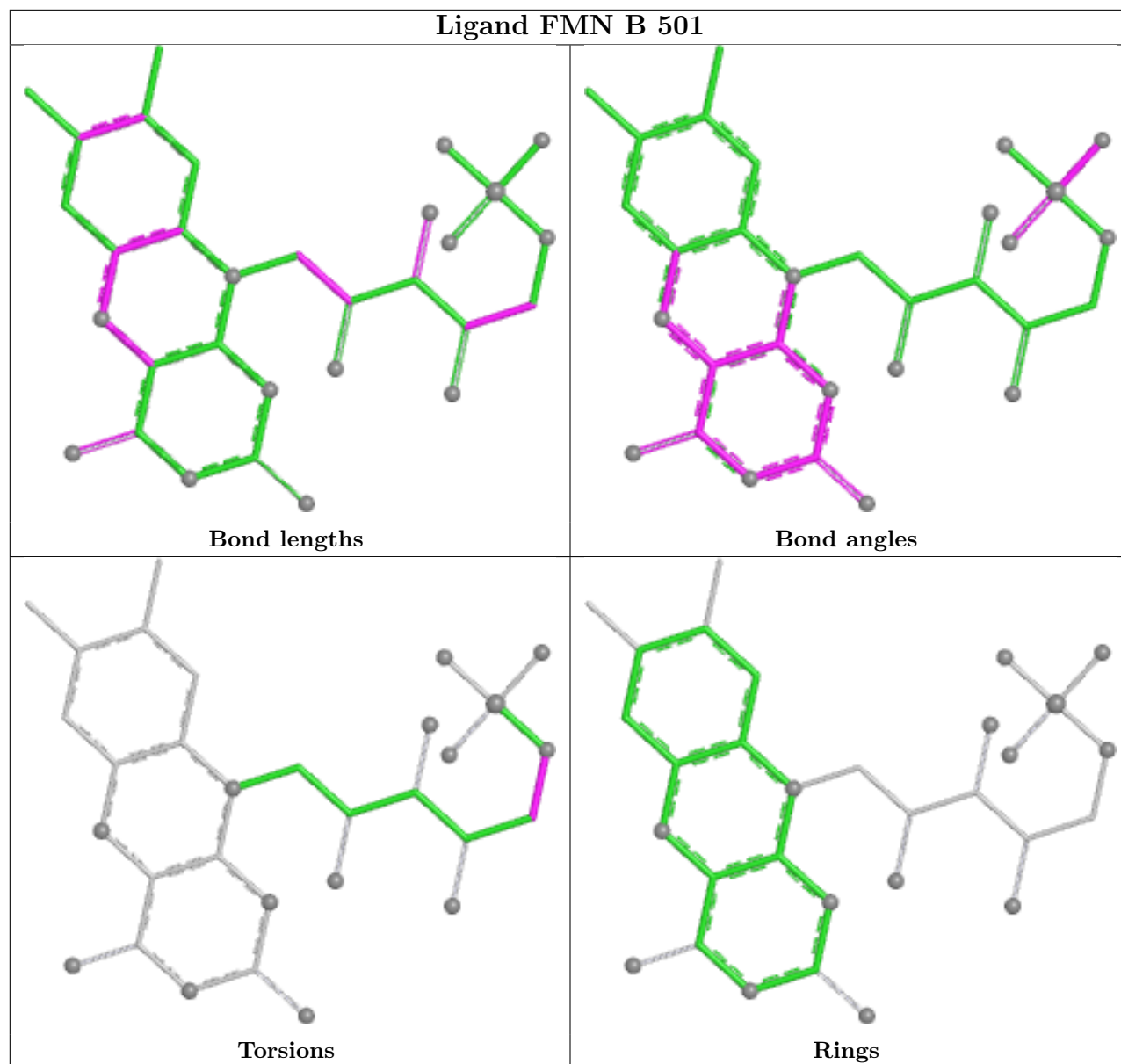
Mol	Chain	Res	Type	Atoms
2	C	501	FMN	C2'-C3'-C4'-O4'
2	A	501	FMN	C4'-C5'-O5'-P
2	B	501	FMN	C4'-C5'-O5'-P
2	D	501	FMN	C4'-C5'-O5'-P
2	C	501	FMN	C4'-C5'-O5'-P

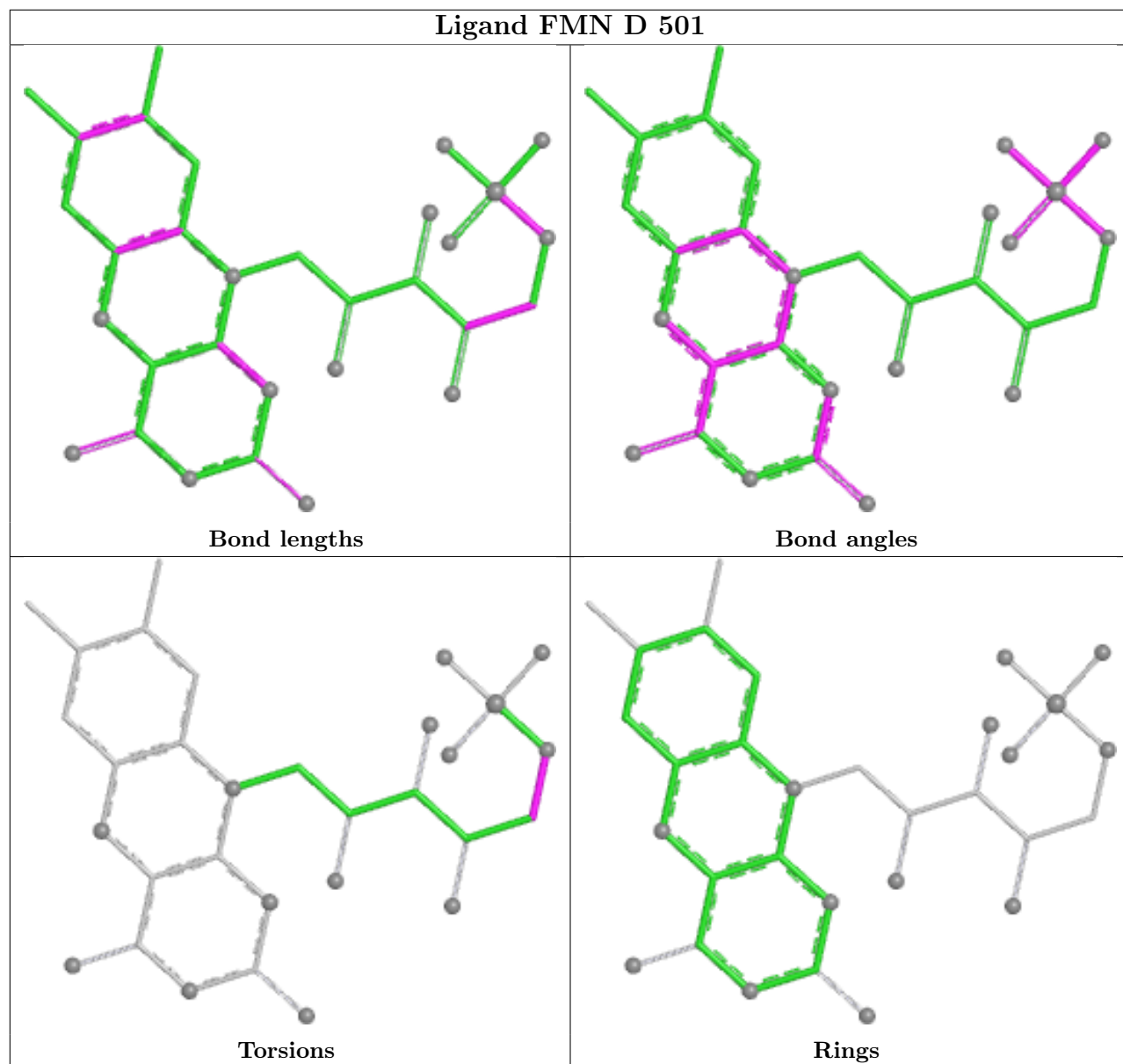
There are no ring outliers.

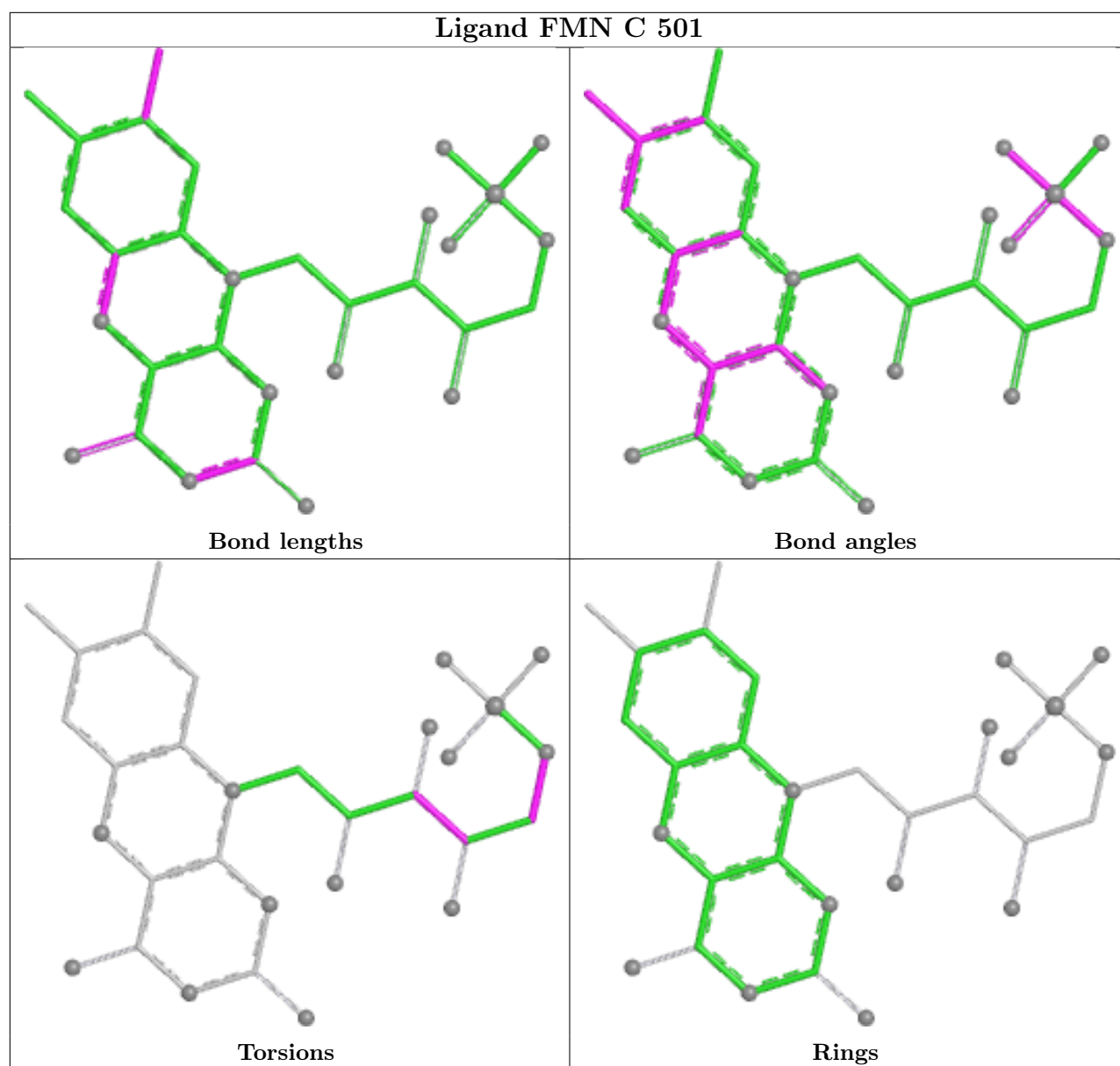
3 monomers are involved in 4 short contacts:

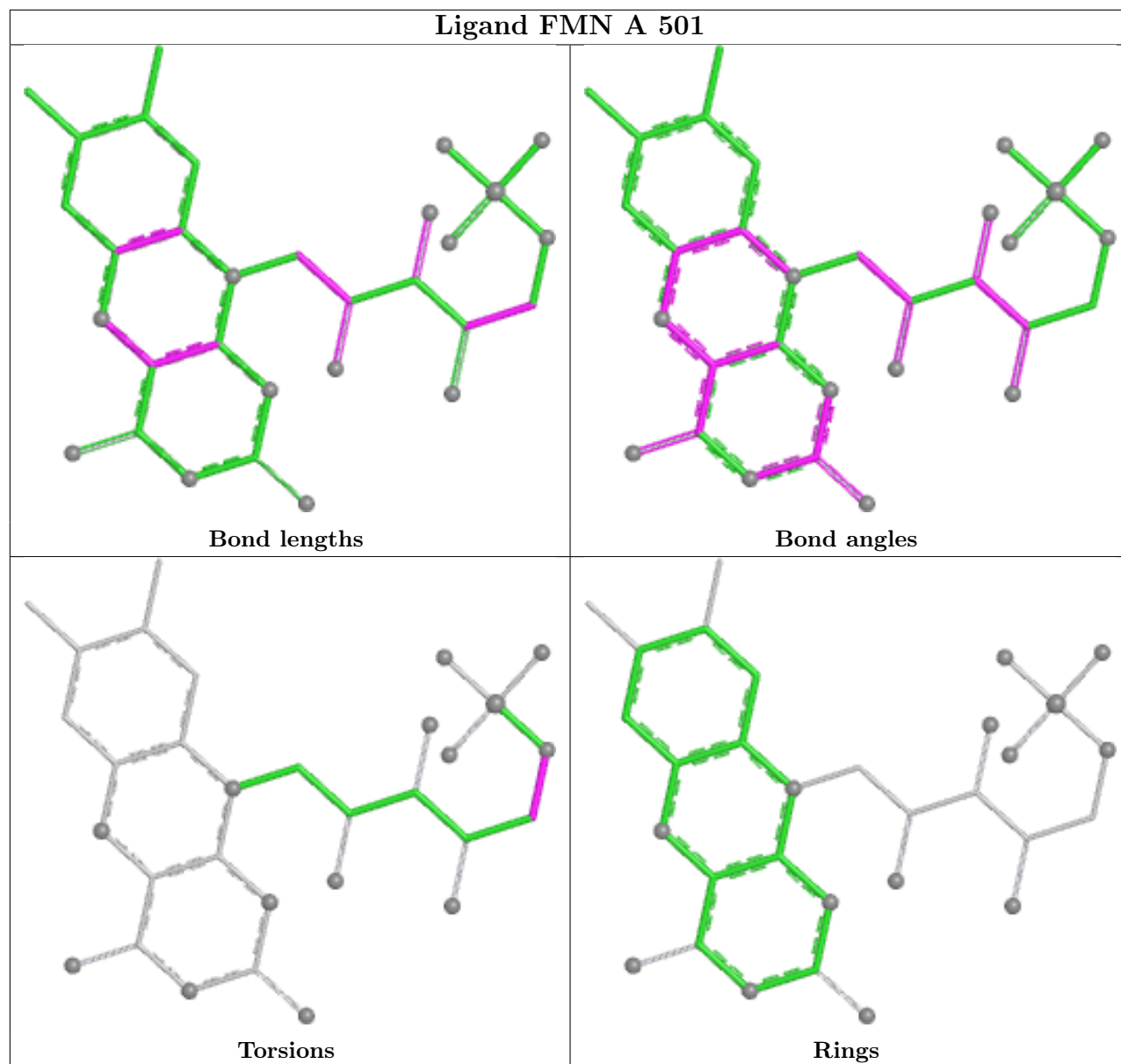
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FMN	1	0
2	D	501	FMN	2	0
2	A	501	FMN	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/403 (99%)	-0.19	1 (0%) 90 90	14, 21, 35, 49	0
1	B	398/403 (98%)	0.02	12 (3%) 52 52	15, 24, 45, 63	0
1	C	399/403 (99%)	-0.04	2 (0%) 87 88	16, 24, 39, 50	0
1	D	396/403 (98%)	6.20	395 (99%) 0 0	49, 83, 121, 145	0
All	All	1592/1612 (98%)	1.49	410 (25%) 1 1	14, 26, 104, 145	0

All (410) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	213	TYR	12.4
1	D	267	TYR	11.8
1	D	74	PHE	11.6
1	D	134	TYR	11.5
1	D	201	PHE	11.4
1	D	85	VAL	11.2
1	D	214	GLY	10.8
1	D	126	VAL	10.4
1	D	154	ALA	10.4
1	D	123	TRP	10.4
1	D	47	ILE	10.2
1	D	89	TRP	10.1
1	D	316	TRP	9.9
1	D	87	GLY	9.9
1	D	136	SER	9.9
1	D	166	ILE	9.9
1	D	161	ILE	9.9
1	D	197	LEU	9.8
1	D	97	TRP	9.8
1	D	174	VAL	9.6
1	D	127	LEU	9.5

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Mol	Chain	Res	Type	RSRZ
1	D	142	TYR	9.5
1	D	183	ALA	9.5
1	D	73	THR	9.5
1	D	181	ILE	9.4
1	D	232	VAL	9.3
1	D	173	TYR	9.3
1	D	118	LEU	9.2
1	D	268	VAL	9.2
1	D	237	ALA	9.2
1	D	116	TRP	9.2
1	D	41	ALA	9.1
1	D	103	ALA	9.1
1	D	100	ILE	9.1
1	D	77	ALA	9.1
1	D	230	ALA	9.1
1	D	42	ILE	9.0
1	D	188	VAL	8.9
1	D	207	ASN	8.9
1	D	152	LEU	8.9
1	D	225	LEU	8.9
1	D	95	ALA	8.9
1	D	224	THR	8.9
1	D	132	LEU	8.8
1	D	236	GLY	8.8
1	D	198	LEU	8.7
1	D	119	GLY	8.7
1	D	104	ILE	8.7
1	D	124	PRO	8.7
1	D	392	VAL	8.6
1	D	169	TYR	8.6
1	D	164	GLU	8.6
1	D	176	ALA	8.6
1	D	185	ALA	8.6
1	D	115	LEU	8.6
1	D	86	PRO	8.6
1	D	135	ASP	8.6
1	D	184	GLY	8.5
1	D	113	VAL	8.5
1	D	157	PRO	8.5
1	D	251	GLY	8.4
1	D	209	ARG	8.4
1	D	377	PHE	8.4

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Mol	Chain	Res	Type	RSRZ
1	D	45	GLY	8.4
1	D	101	PHE	8.3
1	D	283	ALA	8.3
1	D	196	TYR	8.3
1	D	122	ALA	8.2
1	D	199	ASN	8.2
1	D	240	THR	8.2
1	D	117	VAL	8.2
1	D	88	ILE	8.1
1	D	75	PRO	8.1
1	D	284	PHE	8.1
1	D	137	ALA	8.1
1	D	221	ALA	8.1
1	D	205	ILE	8.0
1	D	223	PHE	8.0
1	D	105	HIS	8.0
1	D	177	ALA	8.0
1	D	27	LEU	8.0
1	D	233	ASP	7.9
1	D	50	THR	7.9
1	D	218	GLU	7.9
1	D	131	GLY	7.9
1	D	191	HIS	7.9
1	D	79	SER	7.9
1	D	43	ALA	7.8
1	D	234	ALA	7.8
1	D	151	ALA	7.8
1	D	278	ALA	7.8
1	D	56	TYR	7.8
1	D	170	ILE	7.8
1	D	114	GLN	7.8
1	D	227	VAL	7.8
1	D	270	GLY	7.7
1	D	217	ILE	7.7
1	D	272	LEU	7.7
1	D	159	HIS	7.7
1	D	180	ALA	7.6
1	D	222	ARG	7.6
1	D	175	ASP	7.6
1	D	238	GLU	7.6
1	D	23	GLY	7.5
1	D	212	GLU	7.5

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Mol	Chain	Res	Type	RSRZ
1	D	22	ILE	7.5
1	D	285	ILE	7.5
1	D	228	VAL	7.5
1	D	44	PRO	7.5
1	D	48	PRO	7.5
1	D	206	SER	7.5
1	D	279	GLY	7.5
1	D	158	GLN	7.4
1	D	109	SER	7.4
1	D	40	ARG	7.4
1	D	12	GLY	7.4
1	D	72	GLY	7.3
1	D	76	SER	7.3
1	D	171	LYS	7.3
1	D	229	ASP	7.3
1	D	210	THR	7.3
1	D	193	ALA	7.3
1	D	82	TYR	7.3
1	D	219	ASN	7.3
1	D	160	GLY	7.3
1	D	202	LEU	7.3
1	D	162	THR	7.3
1	D	216	SER	7.3
1	D	242	ILE	7.2
1	D	91	LYS	7.2
1	D	280	LYS	7.2
1	D	235	VAL	7.2
1	D	94	LEU	7.2
1	D	318	GLY	7.2
1	D	231	VAL	7.2
1	D	382	TYR	7.1
1	D	156	ASN	7.1
1	D	315	ILE	7.1
1	D	276	ALA	7.1
1	D	211	ASP	7.1
1	D	244	PHE	7.0
1	D	203	ASP	7.0
1	D	190	ILE	7.0
1	D	138	THR	7.0
1	D	17	PHE	7.0
1	D	80	GLY	7.0
1	D	313	TYR	7.0

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Mol	Chain	Res	Type	RSRZ
1	D	241	SER	6.9
1	D	192	SER	6.9
1	D	110	PHE	6.9
1	D	139	ASP	6.9
1	D	163	LYS	6.9
1	D	250	PHE	6.9
1	D	46	ASN	6.8
1	D	90	SER	6.8
1	D	81	GLY	6.8
1	D	67	LEU	6.8
1	D	263	ALA	6.8
1	D	78	GLN	6.8
1	D	140	ASP	6.8
1	D	69	ILE	6.8
1	D	133	ARG	6.8
1	D	83	PRO	6.7
1	D	68	ILE	6.7
1	D	282	LEU	6.7
1	D	239	ARG	6.7
1	D	102	ASN	6.7
1	D	375	TYR	6.7
1	D	200	GLN	6.7
1	D	49	ASN	6.6
1	D	374	PHE	6.6
1	D	2	SER	6.6
1	D	36	LEU	6.6
1	D	215	GLY	6.5
1	D	334	THR	6.5
1	D	269	ILE	6.5
1	D	343	LEU	6.5
1	D	128	LYS	6.5
1	D	61	SER	6.5
1	D	35	ALA	6.5
1	D	57	TYR	6.5
1	D	112	TRP	6.5
1	D	266	ALA	6.5
1	D	220	ARG	6.4
1	D	24	ASN	6.4
1	D	317	LYS	6.4
1	D	312	ILE	6.4
1	D	342	THR	6.4
1	D	20	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	195	GLY	6.3
1	D	286	ASP	6.3
1	D	320	VAL	6.3
1	D	120	ARG	6.3
1	D	178	LYS	6.3
1	D	179	LYS	6.3
1	D	141	LEU	6.3
1	D	208	ASN	6.3
1	D	396	TYR	6.3
1	D	189	GLN	6.3
1	D	107	ASN	6.3
1	D	150	ARG	6.3
1	D	319	PRO	6.2
1	D	16	ILE	6.2
1	D	93	GLN	6.2
1	D	111	VAL	6.2
1	D	376	THR	6.2
1	D	321	LEU	6.1
1	D	226	GLU	6.1
1	D	51	GLU	6.1
1	D	277	ARG	6.1
1	D	121	GLN	6.1
1	D	99	LYS	6.0
1	D	143	MET	6.0
1	D	130	GLU	6.0
1	D	14	THR	6.0
1	D	383	THR	6.0
1	D	261	ILE	6.0
1	D	358	TYR	6.0
1	D	65	GLY	6.0
1	D	165	GLU	5.9
1	D	271	GLU	5.9
1	D	254	SER	5.9
1	D	314	SER	5.9
1	D	393	ALA	5.9
1	D	288	VAL	5.9
1	D	287	LEU	5.9
1	D	167	LYS	5.8
1	D	13	ASP	5.8
1	D	281	ARG	5.7
1	D	182	ASP	5.7
1	D	53	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	168	GLN	5.7
1	D	52	TRP	5.7
1	D	153	LYS	5.6
1	D	129	LYS	5.6
1	D	253	MET	5.6
1	D	26	GLU	5.5
1	D	187	GLY	5.5
1	D	186	ASP	5.5
1	D	273	GLU	5.5
1	D	37	THR	5.5
1	D	296	PHE	5.5
1	D	365	PRO	5.4
1	D	98	LYS	5.4
1	D	262	VAL	5.4
1	D	155	ASN	5.4
1	D	260	GLY	5.4
1	D	194	ASN	5.4
1	D	292	VAL	5.4
1	D	274	LYS	5.4
1	D	204	PRO	5.4
1	D	96	GLU	5.4
1	D	84	ASN	5.4
1	D	275	ARG	5.4
1	D	252	THR	5.3
1	D	148	LYS	5.3
1	D	31	VAL	5.3
1	D	125	GLU	5.3
1	D	58	ARG	5.3
1	D	144	GLY	5.2
1	D	39	MET	5.2
1	D	106	GLU	5.2
1	D	172	GLU	5.2
1	D	64	PRO	5.2
1	D	340	PRO	5.2
1	D	54	GLU	5.2
1	D	92	GLU	5.2
1	D	264	GLN	5.2
1	D	333	ALA	5.2
1	D	25	ASN	5.1
1	D	66	THR	5.1
1	D	70	THR	5.1
1	D	255	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	354	PRO	5.1
1	D	1	MET	5.0
1	D	323	VAL	5.0
1	D	303	TRP	5.0
1	D	335	LEU	4.9
1	D	265	TYR	4.9
1	D	63	TYR	4.9
1	D	389	GLU	4.8
1	D	363	GLY	4.8
1	D	146	GLU	4.8
1	D	6	PHE	4.8
1	D	293	THR	4.8
1	D	19	PRO	4.8
1	D	8	PRO	4.7
1	D	28	LYS	4.7
1	D	32	VAL	4.7
1	D	59	GLN	4.7
1	D	344	ILE	4.7
1	D	297	LEU	4.7
1	D	356	LEU	4.7
1	D	373	THR	4.7
1	D	18	LYS	4.7
1	D	339	LYS	4.7
1	D	149	GLU	4.6
1	D	357	VAL	4.6
1	D	55	GLU	4.6
1	D	34	PRO	4.6
1	D	29	HIS	4.6
1	D	311	PHE	4.6
1	D	364	LEU	4.5
1	D	108	LYS	4.5
1	D	3	TYR	4.5
1	D	147	GLU	4.5
1	D	15	ASN	4.4
1	D	21	LYS	4.4
1	D	258	ASN	4.4
1	D	304	PHE	4.4
1	D	388	TYR	4.4
1	D	243	ARG	4.4
1	D	249	THR	4.4
1	D	379	LYS	4.3
1	D	346	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	378	THR	4.3
1	D	295	PRO	4.3
1	D	350	PHE	4.3
1	D	245	SER	4.3
1	D	341	ASN	4.2
1	D	248	GLY	4.2
1	D	33	MET	4.1
1	D	11	LEU	4.1
1	D	60	ARG	4.1
1	D	326	TYR	4.0
1	D	299	GLU	4.0
1	D	345	GLY	4.0
1	D	62	GLN	4.0
1	D	352	ALA	4.0
1	D	337	SER	4.0
1	D	38	ARG	3.9
1	D	324	GLY	3.9
1	D	385	TYR	3.9
1	B	303	TRP	3.9
1	D	300	PHE	3.9
1	D	330	PRO	3.8
1	D	381	GLY	3.8
1	D	371	ARG	3.8
1	D	351	ILE	3.8
1	D	145	GLU	3.8
1	D	247	TYR	3.8
1	D	362	LYS	3.8
1	B	304	PHE	3.8
1	D	7	ASP	3.7
1	D	361	GLU	3.7
1	D	355	ASP	3.6
1	D	348	ARG	3.6
1	D	5	ASN	3.6
1	D	256	GLY	3.6
1	D	30	ARG	3.5
1	D	336	ASP	3.5
1	D	368	LYS	3.5
1	D	360	LEU	3.5
1	D	302	LYS	3.4
1	C	1	MET	3.4
1	D	308	THR	3.4
1	D	294	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	289	GLU	3.3
1	D	369	TYR	3.3
1	B	292	VAL	3.3
1	D	71	GLU	3.3
1	D	347	GLY	3.3
1	D	328	LEU	3.3
1	D	307	GLY	3.2
1	D	390	GLU	3.2
1	D	372	ASN	3.1
1	D	386	PRO	3.1
1	D	305	LYS	3.0
1	D	366	LEU	3.0
1	D	395	GLY	3.0
1	D	310	GLU	3.0
1	B	295	PRO	3.0
1	D	246	PRO	3.0
1	D	298	PRO	3.0
1	D	391	SER	2.9
1	D	338	LYS	2.9
1	D	10	PRO	2.9
1	D	331	ASP	2.9
1	D	384	ASP	2.9
1	D	257	GLU	2.9
1	D	325	ASN	2.8
1	D	387	SER	2.8
1	D	353	ASN	2.8
1	D	322	ARG	2.8
1	D	394	LYS	2.8
1	D	359	ARG	2.7
1	D	309	ASN	2.7
1	D	290	PRO	2.7
1	D	349	SER	2.7
1	D	306	GLU	2.7
1	D	370	ASP	2.6
1	D	380	GLU	2.6
1	D	259	PRO	2.5
1	D	329	ASP	2.5
1	B	296	PHE	2.5
1	D	291	ARG	2.5
1	D	367	ASN	2.4
1	B	1	MET	2.4
1	B	298	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	332	GLN	2.3
1	B	300	PHE	2.2
1	B	297	LEU	2.2
1	B	294	ASP	2.2
1	D	4	MET	2.2
1	D	327	ALA	2.1
1	C	2	SER	2.1
1	B	397	LYS	2.1
1	A	50	THR	2.1
1	B	293	THR	2.1
1	D	301	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

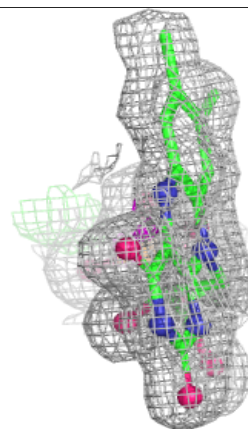
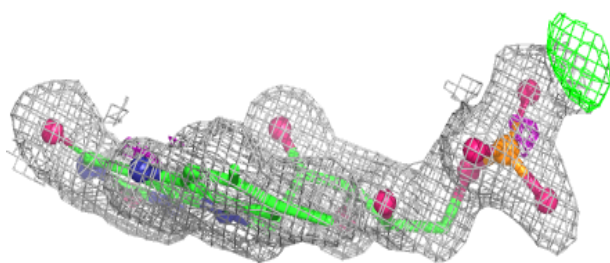
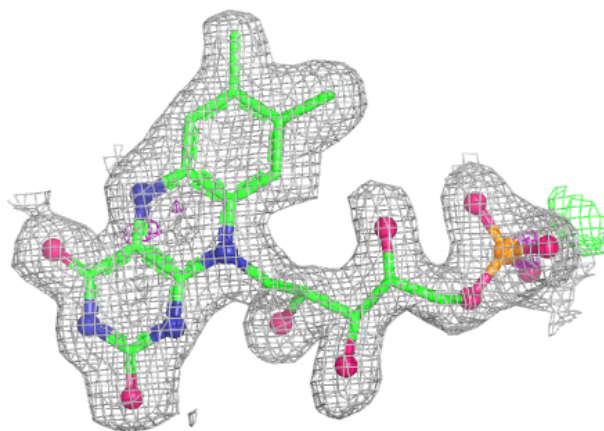
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HBA	B	502	9/9	0.84	0.12	22,31,38,48	0
3	HBA	A	502	9/9	0.86	0.09	21,23,26,35	0
2	FMN	B	501	31/31	0.91	0.09	22,25,29,30	0
3	HBA	C	502	9/9	0.93	0.07	19,21,27,32	0
3	HBA	D	502	9/9	0.93	0.06	21,22,28,33	0
2	FMN	A	501	31/31	0.94	0.07	17,20,22,22	0
2	FMN	D	501	31/31	0.95	0.07	19,22,28,30	0
2	FMN	C	501	31/31	0.97	0.06	17,19,21,22	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.

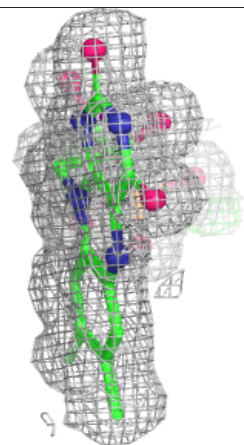
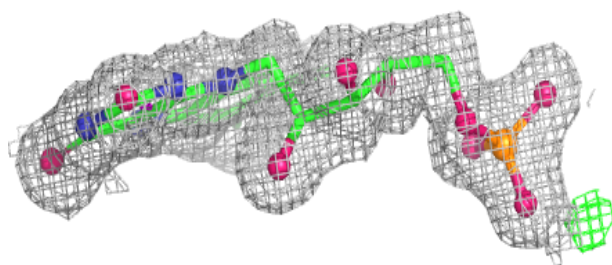
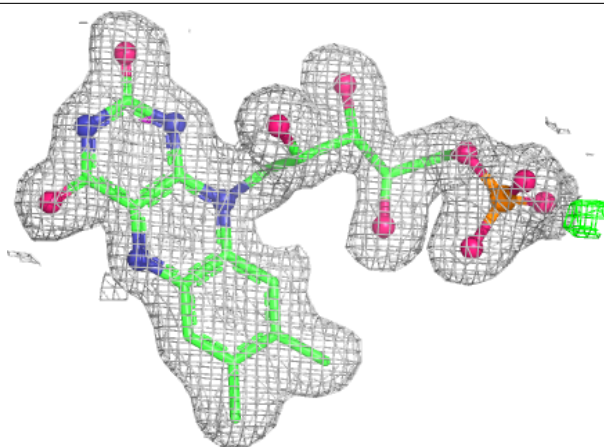
Electron density around FMN B 501:

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



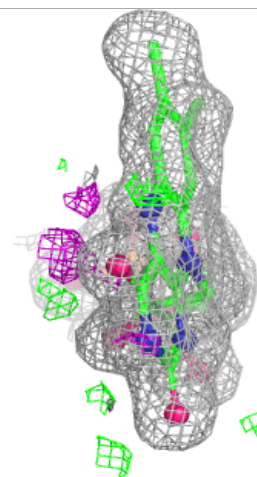
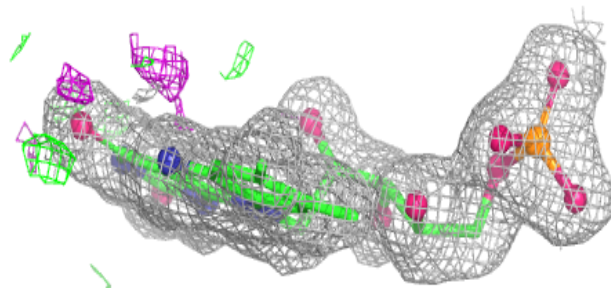
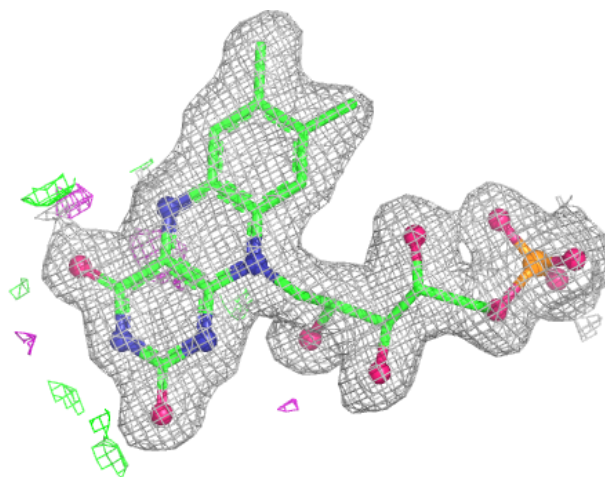
Electron density around FMN A 501:

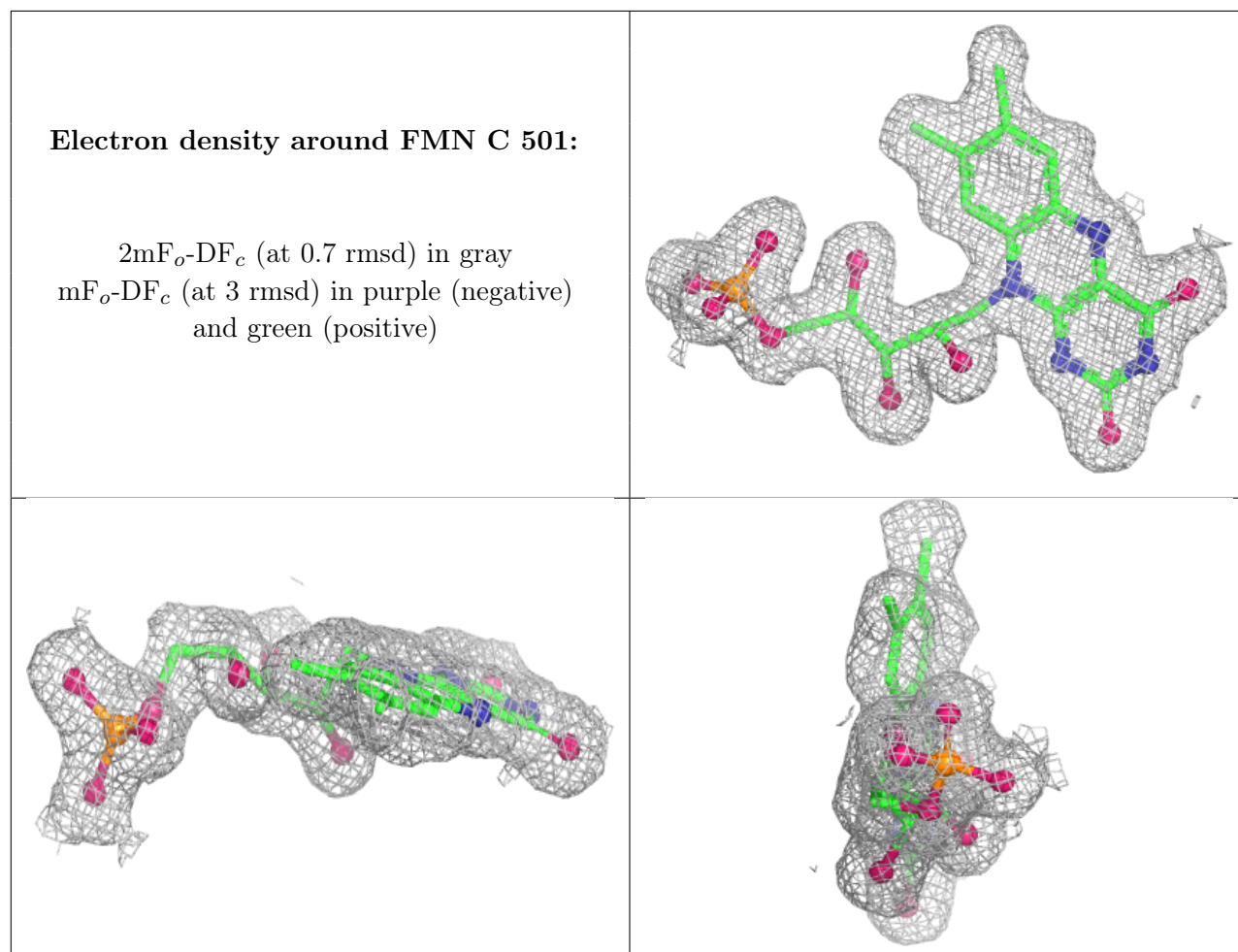
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.