



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:00 PM GMT

PDB ID : 3G5A
Title : Crystal Structure of Candida glabrata FMN Adenylyltransferase in complex with FMN and ATP analog AMPCPP
Authors : Huerta, C.; Zhang, H.
Deposited on : 2009-02-04
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

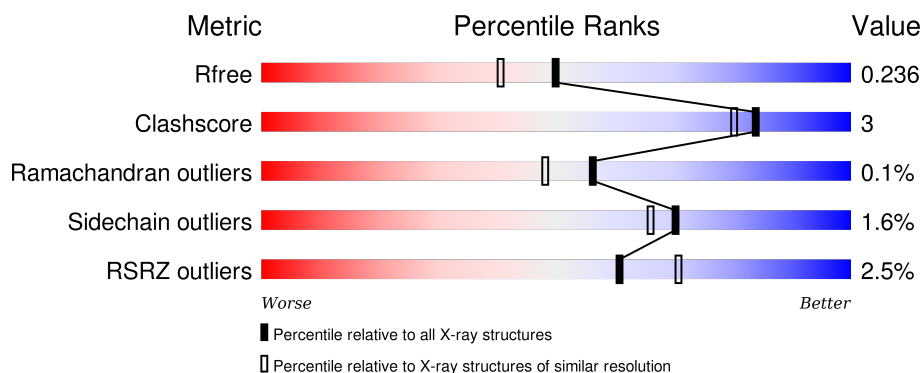
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	308	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	B	308	<div> <div>3%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	C	308	<div> <div>%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	D	308	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>..</div> </div>
1	E	308	<div> <div>2%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	308	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMN	E	306	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16887 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 FMN adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	4	0
			2446	1578	395	464	9			
1	B	305	Total	C	N	O	S	0	2	0
			2529	1634	411	476	8			
1	C	291	Total	C	N	O	S	0	3	0
			2414	1561	388	458	7			
1	D	301	Total	C	N	O	S	0	1	0
			2491	1608	404	472	7			
1	E	286	Total	C	N	O	S	0	2	0
			2371	1531	381	452	7			
1	F	297	Total	C	N	O	S	0	3	0
			2449	1581	395	464	9			

There are 24 discrepancies between the modelled and reference sequences:

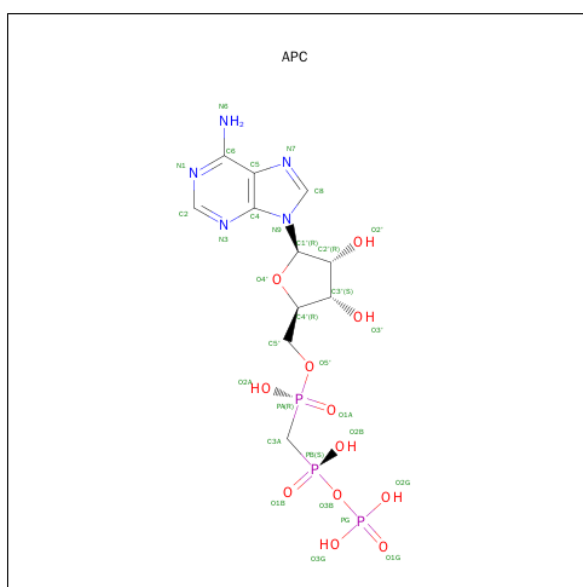
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q6FNA9
A	-2	ALA	-	EXPRESSION TAG	UNP Q6FNA9
A	-1	MET	-	EXPRESSION TAG	UNP Q6FNA9
A	0	VAL	-	EXPRESSION TAG	UNP Q6FNA9
B	-3	GLY	-	EXPRESSION TAG	UNP Q6FNA9
B	-2	ALA	-	EXPRESSION TAG	UNP Q6FNA9
B	-1	MET	-	EXPRESSION TAG	UNP Q6FNA9
B	0	VAL	-	EXPRESSION TAG	UNP Q6FNA9
C	-3	GLY	-	EXPRESSION TAG	UNP Q6FNA9
C	-2	ALA	-	EXPRESSION TAG	UNP Q6FNA9
C	-1	MET	-	EXPRESSION TAG	UNP Q6FNA9
C	0	VAL	-	EXPRESSION TAG	UNP Q6FNA9
D	-3	GLY	-	EXPRESSION TAG	UNP Q6FNA9
D	-2	ALA	-	EXPRESSION TAG	UNP Q6FNA9
D	-1	MET	-	EXPRESSION TAG	UNP Q6FNA9
D	0	VAL	-	EXPRESSION TAG	UNP Q6FNA9
E	-3	GLY	-	EXPRESSION TAG	UNP Q6FNA9

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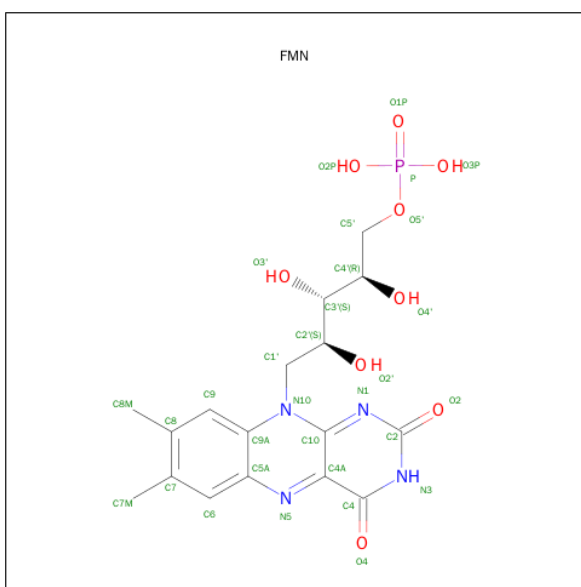
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ALA	-	EXPRESSION TAG	UNP Q6FNA9
E	-1	MET	-	EXPRESSION TAG	UNP Q6FNA9
E	0	VAL	-	EXPRESSION TAG	UNP Q6FNA9
F	-3	GLY	-	EXPRESSION TAG	UNP Q6FNA9
F	-2	ALA	-	EXPRESSION TAG	UNP Q6FNA9
F	-1	MET	-	EXPRESSION TAG	UNP Q6FNA9
F	0	VAL	-	EXPRESSION TAG	UNP Q6FNA9

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			45	13	5	21	6		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

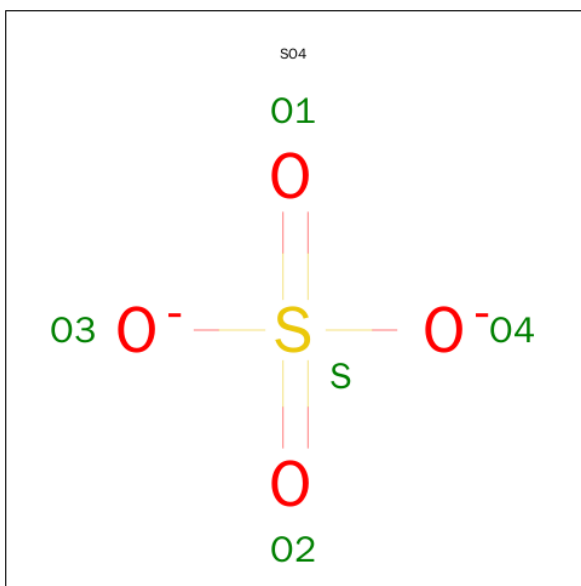


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

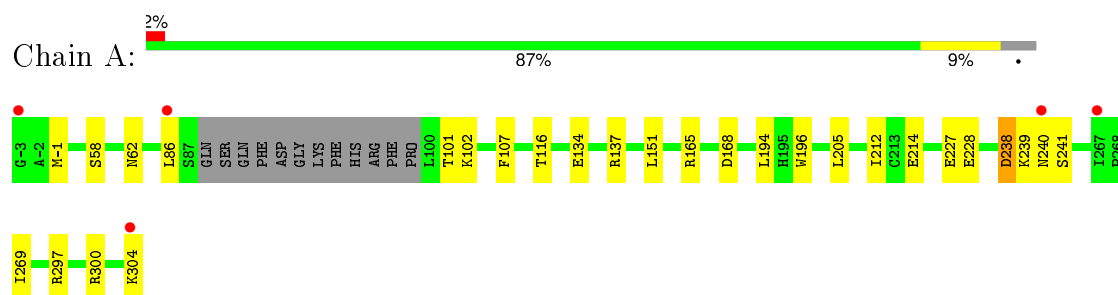
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	316	Total	O	0	0
			316	316		
6	B	311	Total	O	0	0
			311	311		
6	C	311	Total	O	0	0
			311	311		
6	D	285	Total	O	0	0
			285	285		
6	E	269	Total	O	0	0
			269	269		
6	F	298	Total	O	0	0
			298	298		

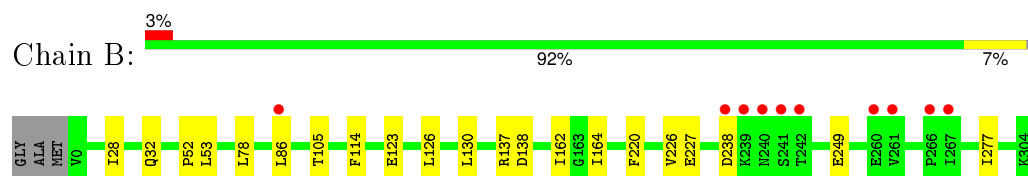
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

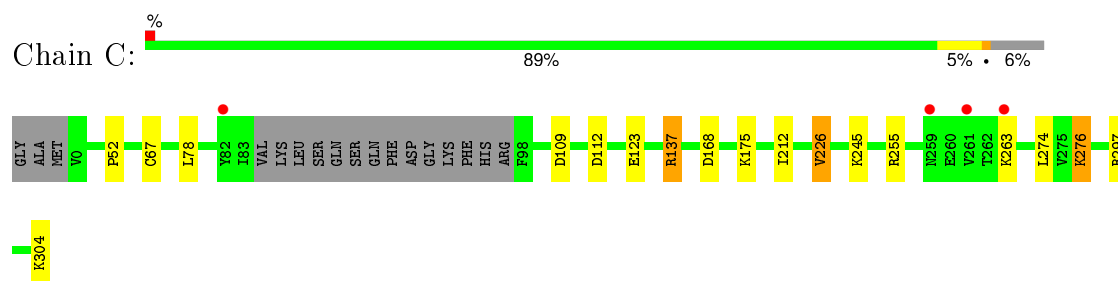
- Molecule 1: FMN adenylyltransferase



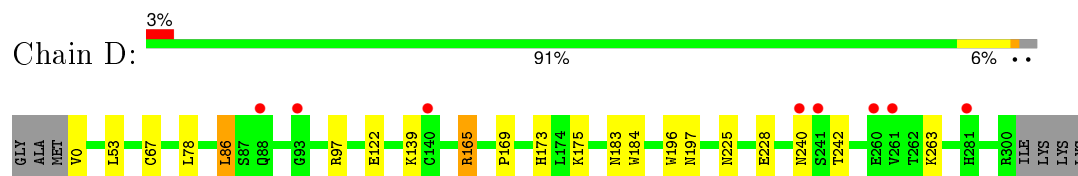
- Molecule 1: FMN adenylyltransferase



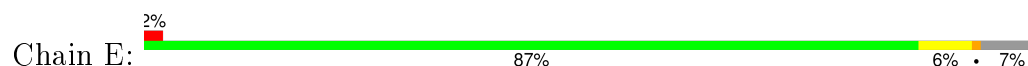
- Molecule 1: FMN adenylyltransferase

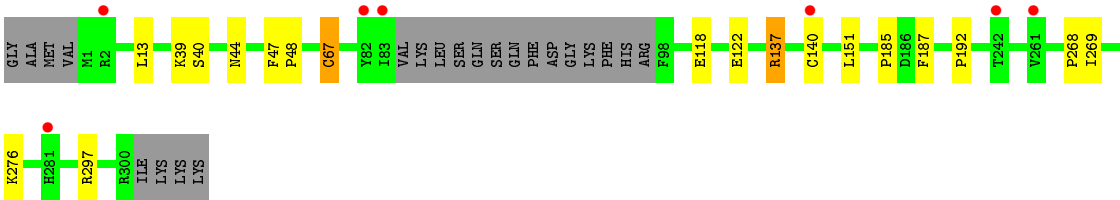


- Molecule 1: FMN adenylyltransferase

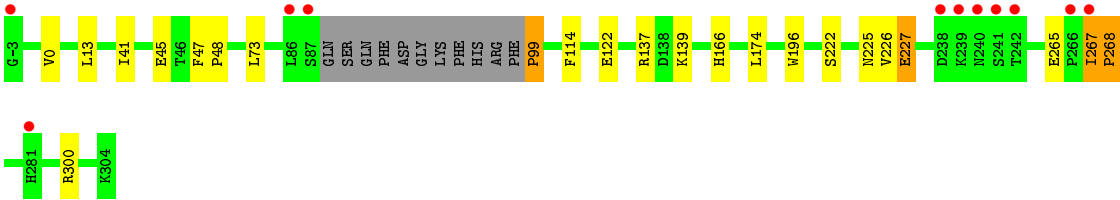
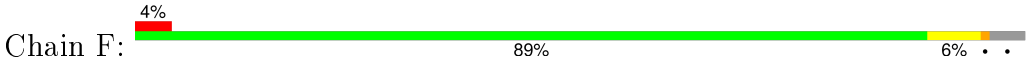


- Molecule 1: FMN adenylyltransferase





● Molecule 1: FMN adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.83 Å 81.75 Å 136.70 Å 90.00° 129.67° 90.00°	Depositor
Resolution (Å)	35.07 – 1.95 34.16 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (35.07-1.95) 96.3 (34.16-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.175 , 0.236 0.175 , 0.236	Depositor DCC
R_{free} test set	6202 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.7	EDS
Estimated twinning fraction	0.013 for -h-2 [*] l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	5 of 123713 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16887	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.01 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0079e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FMN, APC, MG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.71	0/2524	0.69	0/3429
1	B	0.67	0/2605	0.68	0/3539
1	C	0.65	0/2489	0.66	0/3384
1	D	0.68	0/2564	0.69	2/3487 (0.1%)
1	E	0.80	2/2443 (0.1%)	0.67	1/3325 (0.0%)
1	F	0.68	0/2524	0.67	0/3429
All	All	0.70	2/15149 (0.0%)	0.68	3/20593 (0.0%)

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	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	CYS	CB-SG	-23.19	1.42	1.82
1	E	67	CYS	CB-SG	-5.16	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	LEU	CA-CB-CG	7.37	132.25	115.30
1	D	165	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	165	ARG	NE-CZ-NH2	-5.97	117.32	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	267	ILE	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	2446	0	2397	20	0
1	B	2529	0	2473	16	0
1	C	2414	0	2360	14	0
1	D	2491	0	2418	17	0
1	E	2371	0	2297	15	0
1	F	2449	0	2403	13	0
2	A	45	0	10	2	0
2	B	31	0	14	0	0
2	C	31	0	14	1	0
2	D	31	0	14	1	0
2	E	31	0	14	2	0
2	F	31	0	14	0	0
3	A	31	0	19	1	0
3	B	31	0	19	0	0
3	C	31	0	19	1	0
3	D	31	0	19	1	0
3	E	31	0	19	2	0
3	F	31	0	19	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	D	5	0	0	0	0
6	A	316	0	0	4	0
6	B	311	0	0	1	0
6	C	311	0	0	6	0
6	D	285	0	0	4	0
6	E	269	0	0	2	0
6	F	298	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16887	0	14542	88	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 3.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:HIS:HB3	1:E:268:PRO:HG3	1.59	0.85
1:F:99:PRO:HB3	6:F:1685:HOH:O	1.81	0.80
1:D:53:LEU:HD11	1:D:86:LEU:HD21	1.62	0.79
1:B:227:GLU:HG2	1:D:197:ASN:ND2	1.98	0.77
1:F:225:ASN:OD1	1:F:227:GLU:HG3	1.85	0.77
1:C:263:LYS:HG2	6:C:1366:HOH:O	1.85	0.76
1:A:58[B]:SER:OG	6:A:423:HOH:O	2.04	0.75
1:A:304:LYS:HB3	1:C:245:LYS:HZ3	1.53	0.73
1:E:67:CYS:HB3	2:E:305:APC:O3'	1.94	0.68
1:C:168:ASP:OD1	1:C:297:ARG:NH2	2.26	0.68
1:E:118:GLU:OE2	1:E:137:ARG:NH2	2.23	0.67
1:A:240:ASN:HB2	6:A:436:HOH:O	2.00	0.62
3:E:306:FMN:H2'	3:E:306:FMN:H9	1.82	0.61
1:B:53:LEU:HD11	1:B:86:LEU:HD11	1.83	0.61
1:A:304:LYS:HE3	1:C:245:LYS:HD3	1.82	0.61
1:B:114:PHE:HA	1:B:226:VAL:CG1	2.31	0.60
1:D:122:GLU:HG3	6:D:1455:HOH:O	2.03	0.58
1:B:220:PHE:HE2	1:B:277:ILE:HD11	1.66	0.58
3:E:306:FMN:H2'	3:E:306:FMN:C9	2.34	0.58
1:D:184:TRP:HZ2	3:D:306:FMN:HO2'	1.53	0.57
1:A:304:LYS:HB3	1:C:245:LYS:NZ	2.21	0.56
1:D:165:ARG:HD2	1:D:196:TRP:O	2.05	0.56
1:C:175:LYS:HE3	1:F:268:PRO:HG2	1.88	0.55
1:A:116:THR:HG21	1:A:269:ILE:HG22	1.89	0.55
1:C:123:GLU:HG2	6:C:847:HOH:O	2.08	0.53
1:B:227:GLU:HG2	1:D:197:ASN:CG	2.29	0.53
1:B:220:PHE:CE2	1:B:277:ILE:HD11	2.43	0.53
1:B:28:ILE:O	1:B:32:GLN:HG3	2.08	0.53
1:B:114:PHE:CD1	1:B:226:VAL:HG12	2.44	0.53
1:B:162:ILE:HG22	1:B:164:ILE:HG13	1.91	0.53
1:E:297:ARG:HD2	6:E:334:HOH:O	2.08	0.52
1:A:62:ASN:OD1	2:A:305[A]:APC:H3A1	2.09	0.52
1:A:102:LYS:HE3	6:F:1003:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LYS:HE2	1:C:245:LYS:HZ2	1.73	0.52
6:A:1133:HOH:O	1:F:267:ILE:HG21	2.10	0.51
1:D:173:HIS:HB3	1:E:268:PRO:CG	2.38	0.50
1:D:53:LEU:CD1	1:D:86:LEU:HD21	2.36	0.49
1:B:249:GLU:HG2	6:B:414:HOH:O	2.11	0.49
1:A:227:GLU:HG3	6:C:352:HOH:O	2.13	0.48
1:E:39:LYS:HE3	6:E:402:HOH:O	2.13	0.47
1:B:52:PRO:HB2	1:B:78:LEU:HD21	1.96	0.47
1:E:151:LEU:HD11	1:E:187:PHE:CD1	2.48	0.47
1:A:238:ASP:OD1	1:A:241:SER:HB2	2.15	0.47
1:C:304:LYS:HA	6:C:537:HOH:O	2.14	0.47
1:A:101:THR:O	1:A:102:LYS:HD3	2.15	0.46
1:A:168:ASP:OD1	1:A:297:ARG:NH1	2.48	0.46
1:D:0:VAL:N	6:D:449:HOH:O	2.48	0.46
1:C:109:ASP:CG	1:C:137:ARG:HB3	2.36	0.46
1:F:222:SER:HB3	1:F:300:ARG:HH12	1.80	0.46
1:B:138:ASP:CG	1:D:169:PRO:HA	2.35	0.46
1:F:114:PHE:HA	1:F:226:VAL:CG1	2.45	0.46
1:D:225:ASN:ND2	1:D:228:GLU:OE1	2.42	0.46
1:D:175:LYS:HE3	1:E:269:ILE:O	2.17	0.45
1:E:151:LEU:HD11	1:E:187:PHE:HD1	1.82	0.45
1:C:52:PRO:HB2	1:C:78:LEU:HD21	1.99	0.44
1:E:151:LEU:HD12	1:E:185:PRO:HB2	1.99	0.44
1:D:67:CYS:HB3	2:D:305:APC:O3'	2.17	0.44
1:D:240:ASN:HB2	6:D:1368:HOH:O	2.17	0.44
1:A:165:ARG:HA	1:A:194:LEU:HA	1.99	0.43
1:A:205:LEU:HG	1:A:212:ILE:HG21	2.01	0.43
1:C:112:ASP:O	1:C:226:VAL:HG22	2.18	0.43
1:C:67:CYS:HB3	2:C:305:APC:O3'	2.19	0.43
1:A:228:GLU:O	1:A:300:ARG:HA	2.18	0.43
1:A:239:LYS:HB2	1:A:239:LYS:HE3	1.74	0.43
1:E:40:SER:O	1:E:44:ASN:HB2	2.18	0.42
1:D:97:ARG:HD2	6:D:680:HOH:O	2.18	0.42
1:C:276:LYS:HE2	6:C:1118:HOH:O	2.19	0.42
1:B:126:LEU:HD11	1:E:122:GLU:HG3	2.00	0.42
1:E:47:PHE:N	1:E:48:PRO:CD	2.82	0.42
1:D:263:LYS:HE3	1:D:263:LYS:HB2	1.87	0.42
1:A:165:ARG:HD2	1:A:196:TRP:O	2.20	0.42
1:F:41:ILE:O	1:F:45:GLU:HB2	2.19	0.42
2:E:305:APC:H5'2	2:E:305:APC:O1B	2.20	0.42
1:F:166:HIS:HE1	1:F:174:LEU:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:LYS:HE2	1:E:276:LYS:HB2	1.91	0.42
3:C:306:FMN:O3P	6:C:782:HOH:O	2.22	0.41
1:F:47:PHE:N	1:F:48:PRO:CD	2.84	0.41
1:B:123:GLU:HG3	1:E:122:GLU:OE2	2.21	0.41
1:F:139:LYS:HD2	6:F:1195:HOH:O	2.21	0.41
3:A:306:FMN:H1'1	3:A:306:FMN:H9	1.80	0.41
1:F:227:GLU:HG3	1:F:227:GLU:H	1.73	0.41
1:B:114:PHE:CG	1:B:226:VAL:HG12	2.56	0.41
1:A:107:PHE:HD2	1:A:134:GLU:HG2	1.85	0.41
1:F:73:LEU:HD11	1:F:196:TRP:CZ2	2.56	0.41
1:B:105:THR:HG21	1:B:130:LEU:HD13	2.03	0.40
6:A:766:HOH:O	1:F:0:VAL:HG12	2.21	0.40
1:A:214:GLU:HB3	1:A:269:ILE:CG2	2.52	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	296/308 (96%)	290 (98%)	6 (2%)	0	100	100
1	B	305/308 (99%)	302 (99%)	3 (1%)	0	100	100
1	C	290/308 (94%)	289 (100%)	1 (0%)	0	100	100
1	D	300/308 (97%)	298 (99%)	2 (1%)	0	100	100
1	E	284/308 (92%)	277 (98%)	7 (2%)	0	100	100
1	F	296/308 (96%)	289 (98%)	6 (2%)	1 (0%)	46	35
All	All	1771/1848 (96%)	1745 (98%)	25 (1%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	268	PRO

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	274/281 (98%)	269 (98%)	5 (2%)	66	60
1	B	282/281 (100%)	280 (99%)	2 (1%)	88	88
1	C	270/281 (96%)	264 (98%)	6 (2%)	60	51
1	D	277/281 (99%)	272 (98%)	5 (2%)	66	60
1	E	264/281 (94%)	262 (99%)	2 (1%)	86	85
1	F	274/281 (98%)	268 (98%)	6 (2%)	60	51
All	All	1641/1686 (97%)	1615 (98%)	26 (2%)	70	66

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	86	LEU
1	A	137	ARG
1	A	151	LEU
1	A	238	ASP
1	B	137	ARG
1	B	238	ASP
1	C	137	ARG
1	C	212	ILE
1	C	226	VAL
1	C	255	ARG
1	C	274	LEU
1	C	276	LYS
1	D	78	LEU
1	D	86	LEU
1	D	139	LYS
1	D	183	ASN
1	D	242	THR

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Mol	Chain	Res	Type
1	E	137	ARG
1	E	192	PRO
1	F	13	LEU
1	F	99	PRO
1	F	122	GLU
1	F	137	ARG
1	F	227	GLU
1	F	265	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	C	173	HIS
1	D	279	ASN
1	E	279	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	APC	A	305[A]	4	29,33,33	1.99	5 (17%)	29,52,52	2.47	6 (20%)
2	APC	A	305[B]	4	29,33,33	1.17	3 (10%)	29,52,52	2.34	5 (17%)
3	FMN	A	306	-	32,33,33	1.41	5 (15%)	34,50,50	2.24	7 (20%)
2	APC	B	305	4	29,33,33	1.36	3 (10%)	29,52,52	2.43	4 (13%)
3	FMN	B	306	-	32,33,33	1.47	5 (15%)	34,50,50	1.79	8 (23%)
2	APC	C	305	4	29,33,33	1.91	5 (17%)	29,52,52	2.44	7 (24%)
3	FMN	C	306	-	32,33,33	1.42	4 (12%)	34,50,50	1.91	7 (20%)
2	APC	D	305	4	29,33,33	1.42	5 (17%)	29,52,52	1.97	3 (10%)
3	FMN	D	306	-	32,33,33	1.29	4 (12%)	34,50,50	1.91	6 (17%)
5	SO4	D	308	-	4,4,4	0.23	0	6,6,6	0.09	0
2	APC	E	305	4	29,33,33	1.86	6 (20%)	29,52,52	2.27	5 (17%)
3	FMN	E	306	-	32,33,33	1.35	5 (15%)	34,50,50	2.06	9 (26%)
2	APC	F	305	4	29,33,33	1.54	5 (17%)	29,52,52	2.16	4 (13%)
3	FMN	F	306	-	32,33,33	1.46	4 (12%)	34,50,50	1.87	7 (20%)

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	APC	A	305[A]	4	-	0/15/38/38	0/3/3/3
2	APC	A	305[B]	4	-	0/15/38/38	0/3/3/3
3	FMN	A	306	-	-	0/18/18/18	0/3/3/3
2	APC	B	305	4	-	0/15/38/38	0/3/3/3
3	FMN	B	306	-	-	0/18/18/18	0/3/3/3
2	APC	C	305	4	-	0/15/38/38	0/3/3/3
3	FMN	C	306	-	-	0/18/18/18	0/3/3/3
2	APC	D	305	4	-	0/15/38/38	0/3/3/3
3	FMN	D	306	-	-	0/18/18/18	0/3/3/3
5	SO4	D	308	-	-	0/0/0/0	0/0/0/0
2	APC	E	305	4	-	0/15/38/38	0/3/3/3
3	FMN	E	306	-	-	0/18/18/18	0/3/3/3
2	APC	F	305	4	-	0/15/38/38	0/3/3/3
3	FMN	F	306	-	-	0/18/18/18	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	305	APC	PA-O2A	-2.66	1.50	1.56
2	F	305	APC	PB-O2B	-2.64	1.50	1.56
2	E	305	APC	PB-O2B	-2.63	1.50	1.56
2	A	305[B]	APC	PA-O2A	-2.30	1.50	1.56
2	A	305[B]	APC	PB-O2B	-2.23	1.51	1.56
2	F	305	APC	PA-O2A	-2.17	1.51	1.56
2	A	305[A]	APC	PB-O2B	-2.17	1.51	1.56
2	D	305	APC	PB-O2B	-2.10	1.51	1.56
3	A	306	FMN	C10-N1	2.08	1.39	1.35
3	E	306	FMN	C10-N1	2.08	1.39	1.35
3	E	306	FMN	C5A-N5	2.11	1.38	1.35
2	C	305	APC	PA-C3A	2.14	1.82	1.80
3	D	306	FMN	C5A-N5	2.16	1.38	1.35
3	B	306	FMN	C5A-N5	2.21	1.38	1.35
3	B	306	FMN	C10-N1	2.27	1.39	1.35
2	F	305	APC	PA-C3A	2.29	1.82	1.80
2	E	305	APC	C2-N3	2.38	1.36	1.32
3	D	306	FMN	C4A-N5	2.38	1.37	1.33
3	C	306	FMN	C5A-N5	2.45	1.39	1.35
3	A	306	FMN	C4-N3	2.45	1.37	1.33
2	B	305	APC	PA-C3A	2.46	1.82	1.80
2	D	305	APC	PA-C3A	2.59	1.82	1.80
2	D	305	APC	C2-N3	2.68	1.36	1.32
2	B	305	APC	PA-O5'	2.76	1.60	1.57
2	A	305[A]	APC	PA-C3A	2.85	1.83	1.80
3	D	306	FMN	C4-N3	2.98	1.38	1.33
2	A	305[A]	APC	PB-C3A	3.00	1.83	1.80
2	D	305	APC	PA-O5'	3.06	1.60	1.57
3	F	306	FMN	C5A-N5	3.12	1.40	1.35
3	B	306	FMN	C4-N3	3.15	1.38	1.33
2	C	305	APC	O4'-C1'	3.17	1.45	1.41
3	C	306	FMN	C4-N3	3.21	1.38	1.33
3	A	306	FMN	C4A-N5	3.22	1.38	1.33
3	F	306	FMN	C1'-N10	3.26	1.51	1.48
2	E	305	APC	PB-C3A	3.32	1.83	1.80
3	F	306	FMN	C4-N3	3.40	1.39	1.33
3	E	306	FMN	C4-N3	3.46	1.39	1.33
3	A	306	FMN	C5A-N5	3.48	1.40	1.35
3	F	306	FMN	C4A-N5	3.51	1.38	1.33
3	B	306	FMN	C4A-N5	3.53	1.38	1.33
3	E	306	FMN	C4A-N5	3.57	1.38	1.33
3	C	306	FMN	C4A-N5	3.59	1.38	1.33
3	E	306	FMN	C1'-N10	3.65	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	305[A]	APC	PB-O3B	3.65	1.62	1.58
2	A	305[B]	APC	PB-O3B	3.67	1.62	1.58
2	F	305	APC	PA-O5'	3.87	1.61	1.57
3	A	306	FMN	C1'-N10	3.97	1.52	1.48
2	D	305	APC	PB-O3B	3.98	1.62	1.58
3	C	306	FMN	C1'-N10	4.16	1.52	1.48
3	D	306	FMN	C1'-N10	4.18	1.52	1.48
2	B	305	APC	PB-O3B	4.30	1.63	1.58
2	E	305	APC	PB-O3B	4.40	1.63	1.58
2	E	305	APC	PA-C3A	4.47	1.84	1.80
3	B	306	FMN	C1'-N10	4.74	1.53	1.48
2	E	305	APC	PA-O5'	5.04	1.62	1.57
2	F	305	APC	PB-O3B	5.14	1.64	1.58
2	C	305	APC	PB-O3B	5.64	1.64	1.58
2	C	305	APC	PA-O5'	5.77	1.63	1.57
2	A	305[A]	APC	PA-O5'	7.92	1.65	1.57

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	APC	N3-C2-N1	-11.21	120.07	128.87
2	A	305[A]	APC	N3-C2-N1	-10.52	120.60	128.87
2	A	305[B]	APC	N3-C2-N1	-10.52	120.60	128.87
2	E	305	APC	N3-C2-N1	-10.45	120.66	128.87
2	C	305	APC	N3-C2-N1	-10.44	120.67	128.87
2	F	305	APC	N3-C2-N1	-10.08	120.95	128.87
2	D	305	APC	N3-C2-N1	-8.87	121.91	128.87
3	A	306	FMN	N3-C2-N1	-5.83	117.87	127.69
3	C	306	FMN	N3-C2-N1	-4.71	119.76	127.69
3	E	306	FMN	N3-C2-N1	-4.65	119.85	127.69
3	B	306	FMN	N3-C2-N1	-4.49	120.13	127.69
3	F	306	FMN	N3-C2-N1	-4.38	120.32	127.69
3	D	306	FMN	N3-C2-N1	-4.17	120.67	127.69
3	D	306	FMN	C4A-C4-N3	-3.89	118.43	123.52
2	A	305[A]	APC	C5'-C4'-C3'	-3.49	101.69	115.20
3	E	306	FMN	C4A-C4-N3	-3.43	119.04	123.52
3	A	306	FMN	C4A-C4-N3	-3.20	119.34	123.52
2	A	305[B]	APC	O5'-PA-O1A	-3.11	105.45	114.05
2	D	305	APC	O5'-PA-O1A	-3.02	105.71	114.05
2	A	305[A]	APC	O5'-PA-O1A	-2.93	105.95	114.05
3	F	306	FMN	C4A-C4-N3	-2.90	119.73	123.52
3	C	306	FMN	C4A-C4-N3	-2.89	119.75	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	305	APC	O5'-PA-O1A	-2.85	106.17	114.05
2	C	305	APC	O5'-PA-O1A	-2.72	106.53	114.05
2	F	305	APC	C1'-N9-C4	-2.52	124.00	126.81
3	B	306	FMN	C4A-C4-N3	-2.42	120.36	123.52
2	C	305	APC	O2A-PA-O5'	-2.27	100.93	106.69
2	E	305	APC	C1'-N9-C4	-2.19	124.36	126.81
2	B	305	APC	C1'-N9-C4	-2.09	124.47	126.81
2	E	305	APC	O2B-PB-O1B	2.01	116.66	110.24
3	A	306	FMN	O3P-P-O5'	2.02	112.61	106.72
3	D	306	FMN	O2P-P-O5'	2.03	112.66	106.72
2	E	305	APC	O5'-PA-C3A	2.04	110.05	104.23
3	B	306	FMN	C1'-C2'-C3'	2.07	115.73	109.82
3	C	306	FMN	O5'-P-O1P	2.07	112.29	107.08
3	B	306	FMN	O2P-P-O5'	2.13	112.93	106.72
3	E	306	FMN	C4-C4A-N5	2.14	121.30	118.70
2	D	305	APC	O5'-PA-C3A	2.15	110.33	104.23
2	A	305[A]	APC	O2B-PB-O1B	2.18	117.19	110.24
2	F	305	APC	C4'-O4'-C1'	2.21	111.98	109.64
3	F	306	FMN	C4A-N5-C5A	2.21	119.33	116.72
3	D	306	FMN	C4A-N5-C5A	2.21	119.33	116.72
2	A	305[B]	APC	O2B-PB-O1B	2.21	117.30	110.24
3	B	306	FMN	C1'-N10-C9A	2.24	121.42	118.83
3	E	306	FMN	O3'-C3'-C4'	2.29	114.65	108.73
3	E	306	FMN	O2'-C2'-C1'	2.33	115.69	109.93
2	A	305[B]	APC	O2A-PA-O1A	2.34	117.71	110.24
2	F	305	APC	O2A-PA-O1A	2.35	117.74	110.24
3	E	306	FMN	C5A-C9A-N10	2.36	119.34	117.58
3	F	306	FMN	O3P-P-O5'	2.45	113.87	106.72
3	C	306	FMN	C1'-N10-C9A	2.54	121.78	118.83
3	B	306	FMN	C4A-N5-C5A	2.55	119.72	116.72
2	A	305[B]	APC	O2G-PG-O1G	2.57	119.03	110.63
2	C	305	APC	O2B-PB-O1B	2.58	118.49	110.24
3	D	306	FMN	C1'-N10-C9A	2.60	121.84	118.83
2	C	305	APC	O5'-PA-C3A	2.63	111.70	104.23
3	E	306	FMN	C4A-N5-C5A	2.72	119.93	116.72
2	B	305	APC	O2A-PA-O1A	2.78	119.12	110.24
2	C	305	APC	O2A-PA-O1A	2.79	119.16	110.24
3	A	306	FMN	C1'-C2'-C3'	2.79	117.81	109.82
3	C	306	FMN	C4A-N5-C5A	2.84	120.07	116.72
3	A	306	FMN	C4A-N5-C5A	2.89	120.13	116.72
2	C	305	APC	C4'-O4'-C1'	2.99	112.82	109.64
2	A	305[A]	APC	PA-O5'-C5'	3.00	130.80	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	306	FMN	C5A-C9A-N10	3.14	119.93	117.58
3	F	306	FMN	C1'-N10-C9A	3.23	122.58	118.83
3	E	306	FMN	C1'-N10-C9A	3.33	122.69	118.83
2	A	305[A]	APC	O5'-PA-C3A	3.35	113.77	104.23
3	B	306	FMN	C5A-C9A-N10	3.50	120.20	117.58
2	B	305	APC	O3G-PG-O2G	3.61	120.68	107.44
3	A	306	FMN	C5A-C9A-N10	3.66	120.32	117.58
3	C	306	FMN	C5A-C9A-N10	3.80	120.42	117.58
3	B	306	FMN	C4-N3-C2	5.78	119.98	115.16
3	F	306	FMN	C4-N3-C2	6.35	120.45	115.16
3	C	306	FMN	C4-N3-C2	6.51	120.59	115.16
3	E	306	FMN	C4-N3-C2	7.42	121.35	115.16
3	D	306	FMN	C4-N3-C2	7.64	121.53	115.16
3	A	306	FMN	C4-N3-C2	8.76	122.47	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	305[A]	APC	2	0
3	A	306	FMN	1	0
2	C	305	APC	1	0
3	C	306	FMN	1	0
2	D	305	APC	1	0
3	D	306	FMN	1	0
2	E	305	APC	2	0
3	E	306	FMN	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	296/308 (96%)	-0.22	5 (1%) 73 81	6, 14, 29, 40	0
1	B	305/308 (99%)	-0.10	10 (3%) 50 61	8, 16, 35, 54	0
1	C	291/308 (94%)	-0.28	4 (1%) 78 85	8, 16, 30, 42	0
1	D	301/308 (97%)	-0.14	8 (2%) 58 68	8, 16, 33, 43	0
1	E	286/308 (92%)	-0.08	7 (2%) 62 72	10, 19, 33, 49	0
1	F	297/308 (96%)	-0.14	11 (3%) 45 56	6, 16, 31, 50	0
All	All	1776/1848 (96%)	-0.16	45 (2%) 61 71	6, 16, 32, 54	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ASN	6.3
1	E	140	CYS	5.4
1	B	261	VAL	5.2
1	B	242	THR	5.0
1	C	261	VAL	4.8
1	B	241	SER	4.8
1	F	240	ASN	4.4
1	A	267	ILE	4.4
1	F	242	THR	4.1
1	E	281	HIS	4.1
1	D	140	CYS	3.7
1	D	261	VAL	3.6
1	B	260	GLU	3.6
1	F	267	ILE	3.4
1	B	238	ASP	3.4
1	C	82	TYR	3.3
1	F	238	ASP	3.1
1	E	82	TYR	3.0
1	E	261	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	241	SER	2.9
1	D	260	GLU	2.9
1	A	86	LEU	2.9
1	B	239	LYS	2.8
1	F	86	LEU	2.7
1	B	267	ILE	2.6
1	A	240	ASN	2.5
1	C	263	LYS	2.5
1	F	-3	GLY	2.5
1	A	-3	GLY	2.4
1	E	2	ARG	2.4
1	F	266	PRO	2.4
1	F	281	HIS	2.3
1	F	239	LYS	2.3
1	B	266	PRO	2.3
1	D	241	SER	2.3
1	D	93	GLY	2.2
1	E	83	ILE	2.2
1	F	87	SER	2.2
1	B	86	LEU	2.1
1	E	242	THR	2.1
1	C	259	ASN	2.1
1	D	240	ASN	2.0
1	D	281	HIS	2.0
1	A	304	LYS	2.0
1	D	88	GLN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	FMN	E	306	31/31	0.85	0.16	2.78	22,24,35,36	6
3	FMN	B	306	31/31	0.90	0.14	1.75	15,19,34,34	8
3	FMN	C	306	31/31	0.92	0.11	1.12	13,17,27,29	8
3	FMN	D	306	31/31	0.89	0.14	1.04	19,21,32,32	8
5	SO4	D	308	5/5	0.94	0.13	0.70	39,39,40,40	5
3	FMN	A	306	31/31	0.93	0.11	0.61	13,15,25,25	8
2	APC	A	305[A]	31/31	0.97	0.11	0.11	7,9,10,11	14
2	APC	A	305[B]	31/31	0.97	0.11	0.02	7,9,10,11	14
3	FMN	F	306	31/31	0.93	0.10	-0.12	14,17,23,24	8
2	APC	C	305	31/31	0.96	0.08	-0.51	10,13,19,20	0
4	MG	C	307	1/1	0.97	0.09	-0.74	16,16,16,16	0
2	APC	B	305	31/31	0.98	0.08	-0.95	10,11,15,16	0
2	APC	F	305	31/31	0.99	0.07	-1.10	8,10,12,13	0
4	MG	E	307	1/1	0.99	0.07	-1.32	17,17,17,17	0
2	APC	E	305	31/31	0.98	0.07	-1.67	10,13,15,16	0
2	APC	D	305	31/31	0.99	0.07	-1.78	8,12,13,14	0
4	MG	B	307	1/1	0.98	0.04	-1.81	13,13,13,13	0
4	MG	D	307	1/1	1.00	0.04	-1.83	13,13,13,13	0
4	MG	F	307	1/1	0.99	0.05	-1.86	11,11,11,11	0
4	MG	A	307	1/1	1.00	0.03	-2.44	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.