



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:02 AM UTC

PDB ID : 1O94 / pdb_00001o94
Title : Ternary complex between trimethylamine dehydrogenase and electron transferring flavoprotein
Authors : Leys, D.; Basran, J.; Talfournier, F.; Sutcliffe, M.J.; Scrutton, N.S.
Deposited on : 2002-12-11
Resolution : 2.00 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 ⓘ](#)) 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

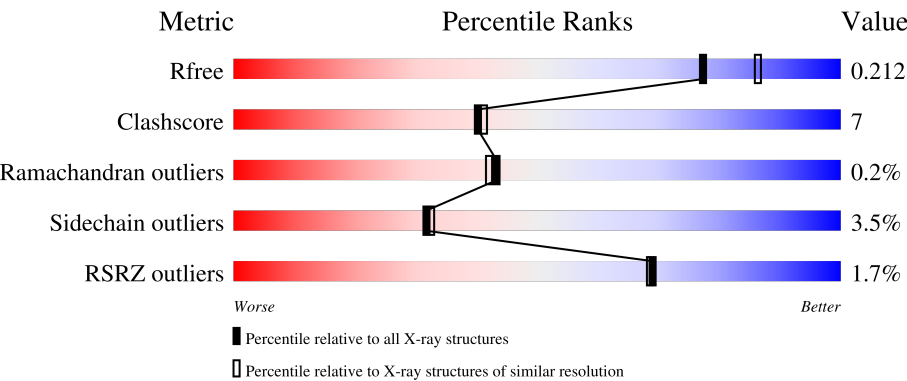
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	729	90%9%
1	B	729	% 88%11%
2	C	264	% 68%16%12%
2	E	264	3% 73%11%11%
3	D	320	6% 48%9%41%

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Mol	Chain	Length	Quality of chain
3	F	320	% 51% 7% 41% ..

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
6	SF4	B	1732	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19925 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 TRIMETHYLAMINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5692	3589	996	1079	28			
1	B	729	Total	C	N	O	S	0	0	0
			5676	3583	994	1071	28			

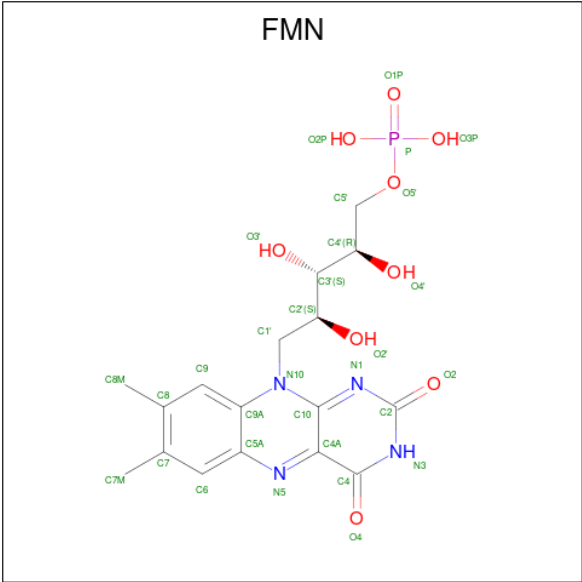
- Molecule 2 is a protein called ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	233	Total	C	N	O	S	0	0	0
			1749	1097	301	341	10			
2	E	236	Total	C	N	O	S	0	0	0
			1751	1102	299	340	10			

- Molecule 3 is a protein called ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT.

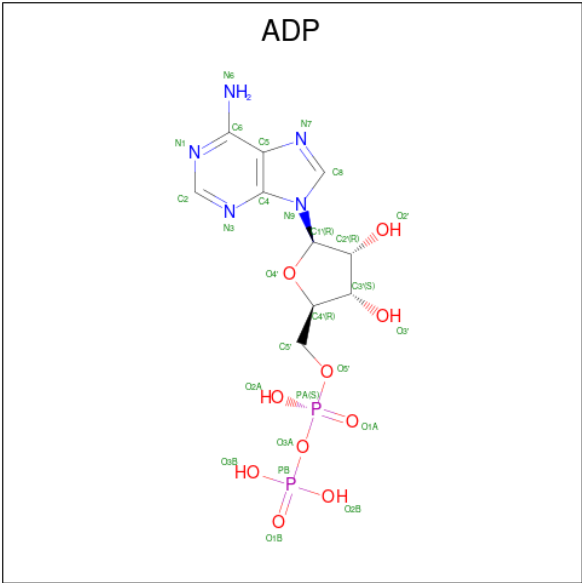
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	189	Total	C	N	O		0	0	0
			1354	857	230	267				
3	F	189	Total	C	N	O		0	0	0
			1376	870	232	274				

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



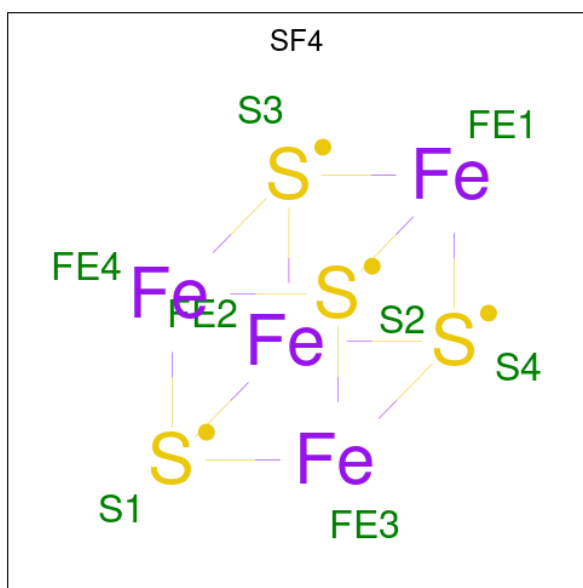
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



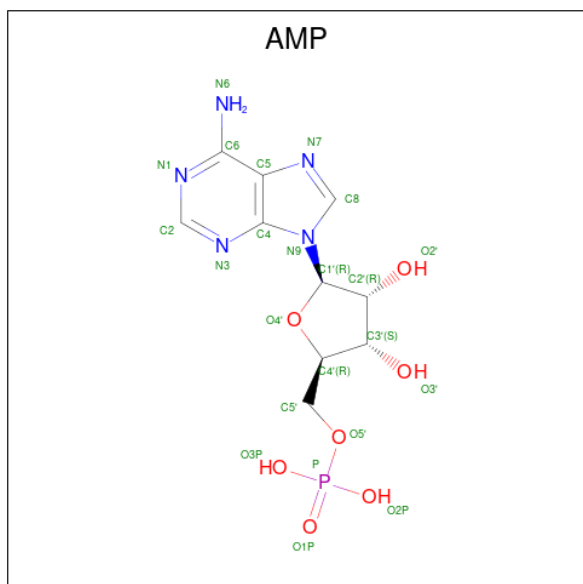
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_7\text{P}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			23	10	5	7		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

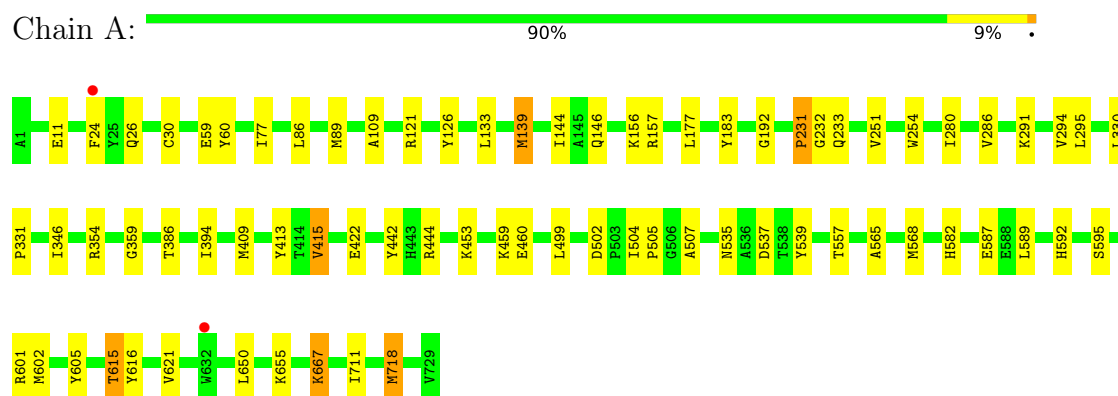
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	718	Total	O	0	0
			718	718		
8	B	831	Total	O	0	0
			831	831		
8	C	178	Total	O	0	0
			178	178		
8	D	73	Total	O	0	0
			73	73		
8	E	198	Total	O	0	0
			198	198		
8	F	151	Total	O	0	0
			151	151		

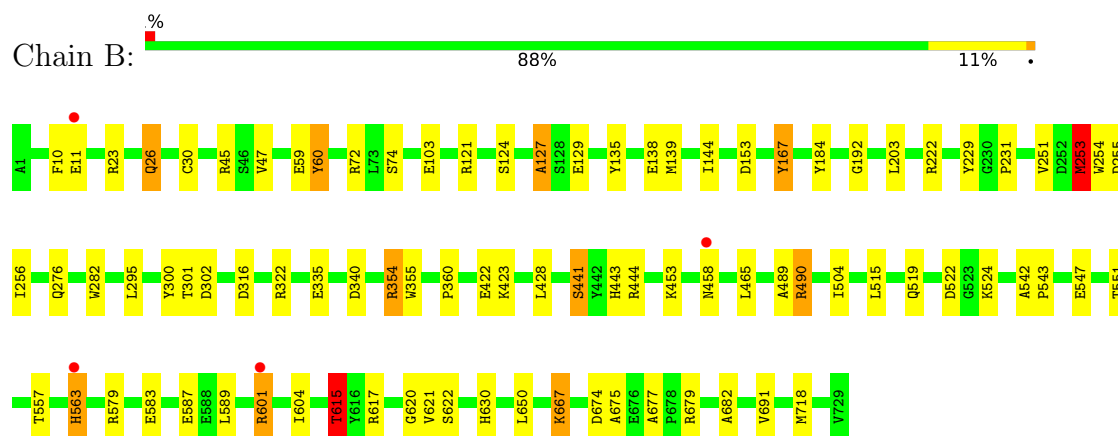
3 Residue-property plots

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.

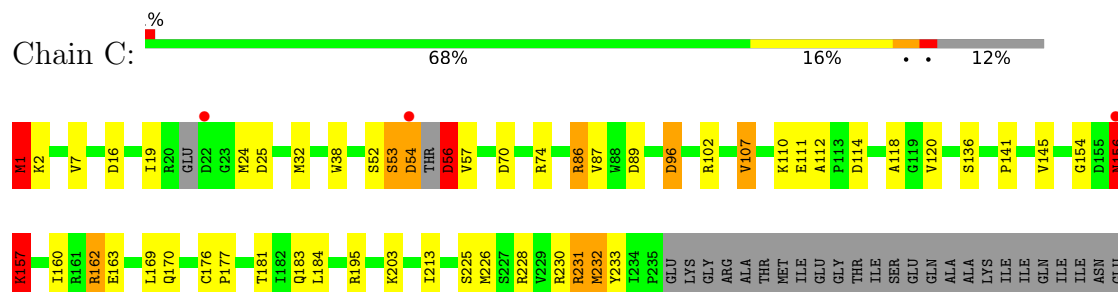
• Molecule 1: TRIMETHYLAMINE DEHYDROGENASE



• Molecule 1: TRIMETHYLAMINE DEHYDROGENASE



• Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.93Å 211.54Å 125.97Å 90.00° 100.03° 90.00°	Depositor
Resolution (Å)	19.88 – 2.00 19.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.88-2.00) 94.7 (19.88-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.08	Depositor
R, R_{free}	0.172 , 0.212 0.175 , 0.212	Depositor DCC
R_{free} test set	9811 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19925	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ADP, SF4, AMP

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	1.25	13/5834 (0.2%)	1.16	12/7918 (0.2%)
1	B	1.32	15/5818 (0.3%)	1.18	12/7902 (0.2%)
2	C	1.45	6/1772 (0.3%)	1.32	16/2402 (0.7%)
2	E	1.20	5/1775 (0.3%)	1.23	10/2408 (0.4%)
3	D	0.88	0/1378	1.06	1/1884 (0.1%)
3	F	1.06	1/1400 (0.1%)	1.23	7/1913 (0.4%)
All	All	1.25	40/17977 (0.2%)	1.19	58/24427 (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	B	0	1
2	C	0	1
3	D	0	1
3	F	0	1
All	All	0	4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	54	ASP	C-N	35.93	1.83	1.33
1	A	568	MET	SD-CE	-10.87	1.52	1.79
1	B	253	MET	SD-CE	10.15	2.04	1.79
2	E	1	MET	SD-CE	-8.88	1.57	1.79
1	A	139	MET	SD-CE	-8.55	1.58	1.79
1	A	409	MET	SD-CE	-8.03	1.59	1.79
2	E	31	MET	SD-CE	-7.80	1.60	1.79
1	B	256	ILE	CA-CB	7.23	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	MET	SD-CE	-7.17	1.61	1.79
1	B	601	ARG	CG-CD	7.16	1.74	1.52
2	E	232	MET	SD-CE	-7.16	1.61	1.79
1	A	504	ILE	CA-C	6.96	1.58	1.52
1	A	539	TYR	CA-C	6.85	1.57	1.53
1	B	675	ALA	CA-CB	6.84	1.64	1.53
1	B	504	ILE	CA-C	6.74	1.58	1.52
2	E	110	LYS	CE-NZ	6.58	1.69	1.49
1	B	677	ALA	CA-CB	6.54	1.63	1.53
1	A	602	MET	SD-CE	6.51	1.95	1.79
2	E	226	MET	SD-CE	-6.43	1.63	1.79
1	B	601	ARG	NE-CZ	6.07	1.39	1.33
2	C	110	LYS	CE-NZ	5.96	1.67	1.49
1	B	192	GLY	CA-C	5.87	1.57	1.52
1	B	679	ARG	CA-C	5.87	1.59	1.52
1	A	565	ALA	CA-CB	5.86	1.62	1.53
2	C	232	MET	SD-CE	-5.84	1.65	1.79
1	A	502	ASP	N-CA	5.79	1.50	1.45
3	F	6	ILE	CA-CB	5.69	1.60	1.53
1	A	711	ILE	C-O	5.68	1.30	1.24
1	A	89	MET	SD-CE	5.58	1.93	1.79
1	A	394	ILE	CA-CB	5.56	1.61	1.54
1	B	563	HIS	CA-CB	5.53	1.61	1.53
1	A	192	GLY	CA-C	5.48	1.57	1.52
1	B	47	VAL	CA-CB	5.45	1.61	1.54
1	B	691	VAL	CA-CB	5.32	1.61	1.54
2	C	112	ALA	CA-CB	5.28	1.56	1.52
1	B	682	ALA	CA-CB	5.28	1.61	1.53
1	B	601	ARG	CD-NE	5.25	1.53	1.46
1	B	153	ASP	N-CA	5.16	1.52	1.46
1	A	507	ALA	CA-CB	5.08	1.60	1.53
2	C	107	VAL	CA-CB	5.02	1.61	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	54	ASP	CA-C-N	18.07	156.06	121.54
2	C	54	ASP	C-N-CA	18.07	156.06	121.54
2	C	156	ASN	N-CA-C	11.13	126.38	113.02
3	F	49	VAL	N-CA-CB	10.76	117.28	110.50
3	F	48	PHE	CA-C-N	-9.11	114.50	120.24
3	F	48	PHE	C-N-CA	-9.11	114.50	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	110	THR	N-CA-C	8.82	124.36	113.50
1	A	157	ARG	NE-CZ-NH1	-8.64	112.86	121.50
1	B	231	PRO	CA-C-N	-8.09	111.05	122.86
1	B	231	PRO	C-N-CA	-8.09	111.05	122.86
2	E	162	ARG	NE-CZ-NH2	-8.01	112.00	119.20
1	B	615	THR	CB-CA-C	-7.29	95.52	109.66
2	E	231	ARG	CB-CA-C	-7.21	96.89	109.86
2	E	16	ASP	N-CA-C	-7.10	91.12	111.00
2	C	54	ASP	N-CA-C	6.96	119.75	108.41
2	C	74	ARG	CG-CD-NE	-6.63	97.41	112.00
2	C	53	SER	N-CA-C	6.60	116.77	108.45
1	A	231	PRO	CA-C-N	-6.50	116.41	123.30
1	A	231	PRO	C-N-CA	-6.50	116.41	123.30
2	E	86	ARG	NE-CZ-NH2	-6.45	113.39	119.20
1	A	157	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	A	232	GLY	N-CA-C	-6.35	106.78	113.58
2	E	162	ARG	NE-CZ-NH1	6.25	127.75	121.50
1	B	153	ASP	N-CA-C	-6.21	104.59	111.36
2	E	86	ARG	CG-CD-NE	-6.19	98.39	112.00
2	C	156	ASN	CA-C-N	6.18	133.35	121.54
2	C	156	ASN	C-N-CA	6.18	133.35	121.54
2	C	157	LYS	N-CA-CB	5.95	120.54	110.49
1	B	620	GLY	N-CA-C	-5.88	107.20	115.32
1	A	415	VAL	N-CA-C	5.88	116.94	108.48
2	C	2	LYS	CB-CG-CD	-5.85	97.85	111.30
1	A	354	ARG	NE-CZ-NH1	-5.76	115.74	121.50
2	C	86	ARG	NE-CZ-NH2	-5.65	114.12	119.20
2	E	203	LYS	N-CA-C	5.62	116.97	109.83
2	E	2	LYS	CB-CG-CD	-5.59	98.44	111.30
2	C	111	GLU	N-CA-C	5.59	118.30	111.82
1	B	322	ARG	N-CA-C	5.54	120.45	113.25
2	E	54	ASP	N-CA-C	-5.42	106.70	113.15
1	A	354	ARG	N-CA-C	5.36	117.54	111.11
1	B	354	ARG	N-CA-C	5.36	116.80	111.07
3	D	146	PRO	N-CA-C	5.35	119.27	111.03
3	F	109	LYS	N-CA-C	5.35	117.11	111.28
1	B	360	PRO	CB-CA-C	-5.33	106.16	111.17
2	C	16	ASP	N-CA-C	-5.32	96.10	111.00
2	C	86	ARG	CG-CD-NE	-5.27	100.40	112.00
1	A	459	LYS	N-CA-C	5.22	118.91	112.54
1	B	47	VAL	N-CA-CB	5.20	117.61	110.54
1	B	127	ALA	N-CA-C	-5.19	100.78	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	ILE	N-CA-C	5.19	115.43	108.17
2	C	156	ASN	O-C-N	-5.18	115.70	122.39
3	F	66	SER	N-CA-C	5.18	117.00	111.36
2	C	162	ARG	CG-CD-NE	5.14	123.30	112.00
3	F	122	GLU	CB-CA-C	-5.12	98.18	109.56
2	E	56	ASP	N-CA-C	5.12	117.89	109.76
1	A	615	THR	OG1-CB-CG2	-5.08	99.13	109.30
1	A	286	VAL	N-CA-C	5.05	115.28	110.53
1	A	453	LYS	N-CA-C	5.04	117.67	111.82
1	B	441	SER	CB-CA-C	-5.04	100.39	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	167	TYR	Peptide
2	C	156	ASN	Peptide
3	D	109	LYS	Peptide
3	F	110	THR	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	5692	0	5444	46	1
1	B	5676	0	5423	62	1
2	C	1749	0	1722	48	1
2	E	1751	0	1716	46	1
3	D	1354	0	1311	26	0
3	F	1376	0	1358	18	0
4	A	31	0	18	0	0
4	B	31	0	18	1	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	8	0	0	0	0
6	B	8	0	0	2	0
7	C	23	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	23	0	12	1	0
8	A	718	0	0	22	0
8	B	831	0	0	31	0
8	C	178	0	0	10	0
8	D	73	0	0	2	0
8	E	198	0	0	13	0
8	F	151	0	0	3	0
All	All	19925	0	17058	230	2

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 7.

All (230) 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)
2:E:110:LYS:CE	2:E:110:LYS:NZ	1.69	1.55
1:B:253:MET:CE	1:B:253:MET:SD	2.04	1.45
1:B:229:TYR:CD1	8:B:2325:HOH:O	1.75	1.35
2:C:54:ASP:C	2:C:56:ASP:N	1.84	1.35
1:A:11:GLU:HG2	8:A:2015:HOH:O	1.31	1.26
1:B:615:THR:HG23	8:B:2680:HOH:O	1.09	1.23
1:B:253:MET:SD	8:B:2230:HOH:O	2.07	1.12
1:B:229:TYR:CB	8:B:2325:HOH:O	1.96	1.11
6:B:1732:SF4:FE3	6:B:1732:SF4:S4	1.42	1.10
1:A:460:GLU:CB	8:A:2457:HOH:O	2.04	1.04
2:E:25:ASP:HA	2:E:232:MET:HE3	1.42	0.98
1:B:11:GLU:HG2	8:B:2012:HOH:O	1.63	0.97
1:B:617:ARG:NE	8:B:2684:HOH:O	1.97	0.96
1:B:229:TYR:HD1	8:B:2325:HOH:O	1.21	0.93
1:A:621:VAL:HB	8:A:2584:HOH:O	1.67	0.93
1:B:422:GLU:HG2	8:B:2500:HOH:O	1.71	0.91
2:E:16:ASP:OD2	8:E:2012:HOH:O	1.87	0.90
2:E:25:ASP:HA	2:E:232:MET:CE	2.03	0.89
1:B:547:GLU:O	1:B:551:THR:HG23	1.76	0.86
2:C:87:VAL:HG21	2:C:107:VAL:HG21	1.57	0.85
1:B:522:ASP:HB3	8:B:2603:HOH:O	1.77	0.84
1:B:229:TYR:HB2	8:B:2325:HOH:O	1.67	0.83
2:C:107:VAL:HG22	2:C:213:ILE:HG21	1.60	0.83
6:B:1732:SF4:FE4	6:B:1732:SF4:S3	1.70	0.82
1:A:422:GLU:CG	8:A:2179:HOH:O	2.31	0.78
2:C:25:ASP:HA	2:C:232:MET:HE3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:LYS:HE3	8:E:2043:HOH:O	1.84	0.76
1:B:524:LYS:CB	8:B:2248:HOH:O	2.34	0.76
1:A:231:PRO:O	8:A:2259:HOH:O	2.03	0.74
2:E:162:ARG:HH11	2:E:170:GLN:NE2	1.83	0.74
2:C:38:TRP:HE1	2:C:183:GLN:NE2	1.87	0.73
2:C:183:GLN:HE21	2:C:184:LEU:H	1.35	0.72
2:C:1:MET:HB2	8:C:2003:HOH:O	1.89	0.72
2:E:25:ASP:CA	2:E:232:MET:HE3	2.21	0.71
2:C:38:TRP:HE1	2:C:183:GLN:HE22	1.37	0.71
2:C:1:MET:CE	8:C:2130:HOH:O	2.40	0.70
2:C:228:ARG:HD3	3:D:144:ASP:OD1	1.92	0.70
2:E:225:SER:CB	8:E:2103:HOH:O	2.39	0.70
1:A:621:VAL:CB	8:A:2584:HOH:O	2.34	0.69
1:B:490:ARG:HD3	8:B:2566:HOH:O	1.90	0.69
2:C:230:ARG:HH22	3:D:124:GLN:NE2	1.90	0.69
2:C:231:ARG:HH12	3:D:142:GLU:CD	2.02	0.68
2:E:218:ASN:C	8:E:2191:HOH:O	2.35	0.68
2:E:1:MET:HE3	8:E:2116:HOH:O	1.94	0.67
1:A:291:LYS:NZ	8:A:2325:HOH:O	2.26	0.67
1:A:667:LYS:HD2	8:A:2483:HOH:O	1.94	0.67
1:B:615:THR:CG2	8:B:2680:HOH:O	1.90	0.67
2:C:230:ARG:HD3	3:D:144:ASP:OD2	1.95	0.67
2:C:87:VAL:CG2	2:C:107:VAL:HG21	2.25	0.66
2:C:230:ARG:HH22	3:D:124:GLN:HE22	1.42	0.66
1:B:622:SER:CA	8:B:2690:HOH:O	2.45	0.65
1:A:718:MET:HG2	8:A:2284:HOH:O	1.95	0.65
2:C:24:MET:CB	8:C:2173:HOH:O	2.44	0.65
2:C:102:ARG:HH11	2:C:102:ARG:HG3	1.61	0.65
2:E:230:ARG:HH22	3:F:124:GLN:NE2	1.96	0.64
1:B:615:THR:CB	8:B:2680:HOH:O	2.32	0.63
1:B:276:GLN:HE22	1:B:302:ASP:H	1.46	0.63
2:C:1:MET:HE2	2:C:114:ASP:CG	2.24	0.63
2:E:156:ASN:HB2	8:E:2146:HOH:O	1.97	0.63
1:B:124:SER:HA	1:B:138:GLU:HG3	1.81	0.62
1:A:582:HIS:HD2	8:B:2665:HOH:O	1.83	0.62
3:F:49:VAL:HG22	3:F:50:PRO:HD3	1.80	0.62
1:B:579:ARG:O	1:B:583:GLU:HG3	1.99	0.62
2:E:162:ARG:HH11	2:E:170:GLN:HE22	1.46	0.62
3:F:83:ILE:HD13	3:F:150:THR:HG21	1.80	0.61
2:C:226:MET:CE	3:D:111:GLY:HA2	2.31	0.61
2:C:226:MET:HE2	3:D:111:GLY:HA2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:219:ASP:N	8:E:2191:HOH:O	2.34	0.61
1:A:156:LYS:HD2	8:A:2172:HOH:O	2.00	0.60
2:E:28:GLU:HA	2:E:31:MET:HE2	1.83	0.60
1:A:156:LYS:CE	8:A:2172:HOH:O	2.48	0.60
1:B:139:MET:HE2	1:B:144:ILE:HA	1.83	0.60
2:E:1:MET:CE	8:E:2116:HOH:O	2.48	0.60
2:E:58:GLU:OE2	2:E:83:ARG:HD3	2.02	0.60
2:E:1:MET:HG2	2:E:57:VAL:HG22	1.84	0.60
1:B:30:CYS:HA	1:B:59:GLU:HB3	1.83	0.59
3:D:109:LYS:HB2	3:D:110:THR:HG23	1.84	0.59
1:B:551:THR:HG21	8:B:2621:HOH:O	2.03	0.59
1:B:251:VAL:HG21	1:B:254:TRP:CE2	2.38	0.59
2:E:24:MET:O	2:E:232:MET:HE3	2.03	0.59
1:A:718:MET:HE3	8:A:2284:HOH:O	2.02	0.58
1:B:667:LYS:HD2	8:B:2738:HOH:O	2.02	0.58
2:C:231:ARG:NH1	3:D:142:GLU:CD	2.60	0.58
2:E:226:MET:HE3	3:F:148:LYS:HZ1	1.68	0.58
1:B:276:GLN:HE21	1:B:300:TYR:HA	1.68	0.58
2:E:183:GLN:HE21	2:E:184:LEU:H	1.53	0.57
3:F:137:GLN:NE2	3:F:156:ARG:HH22	2.03	0.56
3:D:17:VAL:HG22	3:D:21:LEU:HD23	1.86	0.56
1:A:24:PHE:CD1	1:A:331:PRO:HB3	2.41	0.56
2:E:226:MET:HE3	3:F:148:LYS:NZ	2.21	0.56
2:C:25:ASP:HA	2:C:232:MET:CE	2.34	0.56
2:E:162:ARG:HD3	2:E:170:GLN:HE21	1.71	0.56
3:D:65:GLY:HA3	8:D:2025:HOH:O	2.06	0.56
2:C:136:SER:HB2	3:D:105:SER:HB2	1.87	0.55
1:B:127:ALA:HB2	1:B:135:TYR:CE1	2.41	0.55
1:A:499:LEU:CD2	8:B:2151:HOH:O	2.53	0.55
1:B:276:GLN:NE2	1:B:301:THR:H	2.05	0.55
2:C:226:MET:HE3	2:C:226:MET:HA	1.89	0.55
2:E:230:ARG:HH12	3:F:124:GLN:HE22	1.55	0.55
2:E:171:GLU:OE2	8:E:2152:HOH:O	2.18	0.54
1:B:251:VAL:HG21	1:B:254:TRP:NE1	2.23	0.54
7:E:1237:AMP:H5'1	8:E:2117:HOH:O	2.08	0.54
2:E:1:MET:HE1	2:E:154:GLY:H	1.73	0.54
1:A:386:THR:HB	1:A:413:TYR:CZ	2.43	0.54
1:B:229:TYR:CA	8:B:2325:HOH:O	2.47	0.54
1:B:103:GLU:HA	1:B:167:TYR:HB2	1.90	0.53
1:B:557:THR:HG23	1:B:587:GLU:HG2	1.90	0.53
3:D:19:LEU:HA	3:D:22:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:CYS:H	4:B:1730:FMN:C5A	2.21	0.53
1:A:535:ASN:ND2	1:A:537:ASP:H	2.07	0.52
1:B:295:LEU:C	1:B:295:LEU:HD12	2.34	0.52
2:C:162:ARG:HE	2:C:170:GLN:HE21	1.58	0.52
3:F:180:GLN:NE2	3:F:181:SER:O	2.42	0.52
3:F:11:ARG:O	3:F:12:ASN:HB2	2.08	0.52
2:E:38:TRP:HE1	2:E:183:GLN:NE2	2.08	0.52
1:A:557:THR:HG23	1:A:587:GLU:HG2	1.91	0.52
1:A:601:ARG:CD	8:A:2566:HOH:O	2.58	0.52
2:E:230:ARG:HH22	3:F:124:GLN:HE22	1.58	0.51
1:A:621:VAL:CG2	8:A:2584:HOH:O	2.57	0.51
1:B:615:THR:CA	8:B:2680:HOH:O	2.57	0.51
1:B:587:GLU:HB2	8:B:2648:HOH:O	2.10	0.51
2:E:232:MET:HG2	3:F:141:VAL:HG22	1.93	0.51
2:C:96:ASP:HB3	2:C:225:SER:OG	2.10	0.50
2:C:53:SER:CB	8:C:2058:HOH:O	2.60	0.50
1:A:621:VAL:HG22	8:A:2586:HOH:O	2.11	0.49
1:A:499:LEU:HD23	8:B:2151:HOH:O	2.11	0.49
2:C:231:ARG:NH1	3:D:142:GLU:OE1	2.45	0.49
2:E:1:MET:HG3	2:E:2:LYS:N	2.22	0.49
1:B:253:MET:CE	1:B:253:MET:HB3	2.42	0.49
2:C:232:MET:HG2	3:D:141:VAL:HG22	1.95	0.49
2:C:231:ARG:HH11	2:C:231:ARG:HB3	1.77	0.49
3:D:11:ARG:O	3:D:12:ASN:HB2	2.13	0.49
2:E:226:MET:HE3	2:E:226:MET:HA	1.95	0.49
1:A:156:LYS:CD	8:A:2172:HOH:O	2.59	0.48
1:A:156:LYS:HE3	8:A:2172:HOH:O	2.09	0.48
1:A:251:VAL:HG21	1:A:254:TRP:CE2	2.48	0.48
1:A:254:TRP:HB2	1:A:294:VAL:HG22	1.95	0.48
1:A:346:ILE:HG22	1:A:442:TYR:HB2	1.95	0.48
1:A:616:TYR:HD2	1:B:282:TRP:CE2	2.31	0.48
2:E:28:GLU:HA	2:E:31:MET:CE	2.43	0.48
3:D:76:GLU:CD	3:D:105:SER:HG	2.22	0.48
1:A:280:ILE:HD12	8:A:2334:HOH:O	2.13	0.48
2:E:226:MET:CE	3:F:148:LYS:NZ	2.77	0.48
3:D:17:VAL:HG22	3:D:21:LEU:CD2	2.44	0.47
2:E:121:GLN:NE2	8:E:2119:HOH:O	2.44	0.47
2:E:79:LYS:NZ	8:E:2090:HOH:O	2.47	0.47
1:B:428:LEU:HD21	1:B:443:HIS:HB3	1.97	0.47
2:C:154:GLY:HA2	8:C:2130:HOH:O	2.14	0.47
3:D:76:GLU:CD	3:D:105:SER:OG	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:TYR:CE2	1:B:74:SER:HA	2.49	0.47
1:B:129:GLU:OE2	1:B:184:TYR:OH	2.31	0.47
1:B:617:ARG:NH2	8:B:2685:HOH:O	2.48	0.46
1:A:621:VAL:HG23	8:A:2584:HOH:O	2.15	0.46
3:D:91:VAL:HG13	3:D:152:VAL:HG22	1.96	0.46
2:E:157:LYS:CE	2:E:175:ASN:ND2	2.79	0.46
2:E:157:LYS:HE2	2:E:175:ASN:ND2	2.31	0.46
1:A:592:HIS:HA	1:A:605:TYR:O	2.15	0.46
1:B:23:ARG:HD3	1:B:316:ASP:O	2.16	0.46
2:C:19:ILE:CD1	2:C:233:TYR:HA	2.46	0.46
2:C:54:ASP:CA	2:C:56:ASP:N	2.73	0.46
1:B:423:LYS:HA	1:B:465:LEU:HD13	1.96	0.46
1:B:253:MET:CE	1:B:253:MET:CB	2.94	0.46
2:E:38:TRP:HE1	2:E:183:GLN:HE22	1.64	0.46
2:C:162:ARG:HE	2:C:170:GLN:NE2	2.14	0.45
3:F:64:LYS:HG3	8:F:2042:HOH:O	2.16	0.45
1:A:77:ILE:HD13	1:A:86:LEU:HD12	1.97	0.45
7:C:1236:AMP:H5'1	8:C:2114:HOH:O	2.15	0.45
1:B:354:ARG:HD3	1:B:354:ARG:HA	1.65	0.45
2:C:176:CYS:HA	2:C:177:PRO:C	2.41	0.45
1:A:30:CYS:HA	1:A:59:GLU:HB3	1.98	0.45
2:C:96:ASP:HB3	2:C:225:SER:CB	2.46	0.45
1:A:139:MET:HE2	1:A:144:ILE:CG1	2.47	0.45
2:C:195:ARG:NH1	8:C:2156:HOH:O	2.49	0.45
1:B:340:ASP:OD2	1:B:453:LYS:NZ	2.50	0.45
2:E:102:ARG:O	2:E:102:ARG:HG3	2.13	0.45
1:B:11:GLU:CG	8:B:2012:HOH:O	2.41	0.44
3:F:114:PHE:HA	3:F:152:VAL:O	2.17	0.44
1:B:26:GLN:HE22	1:B:45:ARG:HH21	1.65	0.44
1:A:133:LEU:CD2	8:B:2615:HOH:O	2.66	0.44
2:C:1:MET:HG2	2:C:57:VAL:HG22	2.00	0.44
3:D:122:GLU:OE2	3:D:124:GLN:HG2	2.18	0.44
3:F:66:SER:HB2	8:F:2063:HOH:O	2.18	0.44
1:B:222:ARG:HA	1:B:255:ASP:O	2.18	0.44
1:B:139:MET:CE	1:B:144:ILE:HA	2.46	0.43
2:E:19:ILE:CD1	2:E:233:TYR:HA	2.47	0.43
1:B:604:ILE:O	1:B:630:HIS:HA	2.18	0.43
2:C:52:SER:CB	8:C:2049:HOH:O	2.66	0.43
1:A:11:GLU:CG	8:A:2015:HOH:O	2.16	0.43
1:A:109:ALA:HB3	1:A:126:TYR:CE2	2.53	0.43
2:E:230:ARG:NH2	3:F:124:GLN:NE2	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:17:VAL:O	3:D:21:LEU:HD23	2.19	0.43
3:D:137:GLN:NE2	3:D:156:ARG:HH22	2.15	0.43
1:B:10:PHE:CE2	1:B:335:GLU:HB2	2.53	0.43
2:C:96:ASP:HB3	2:C:225:SER:HB3	2.01	0.43
2:E:228:ARG:CD	8:F:2110:HOH:O	2.67	0.42
1:A:121:ARG:HH22	1:A:146:GLN:NE2	2.18	0.42
1:B:121:ARG:HB3	1:B:139:MET:CG	2.48	0.42
2:C:141:PRO:HD2	2:C:177:PRO:O	2.19	0.42
3:F:49:VAL:CG2	3:F:50:PRO:HD3	2.49	0.42
1:B:615:THR:OG1	8:B:2681:HOH:O	2.20	0.42
2:C:1:MET:HE1	8:C:2130:HOH:O	2.12	0.42
2:C:118:ALA:O	2:C:181:THR:HA	2.18	0.42
1:A:655:LYS:NZ	8:A:2627:HOH:O	2.52	0.42
2:E:40:ASP:OD2	2:E:79:LYS:HE2	2.19	0.42
1:B:458:ASN:HB2	8:B:2488:HOH:O	2.20	0.42
1:A:183:TYR:HB2	1:A:233:GLN:HG2	2.01	0.42
1:B:489:ALA:HB2	1:B:674:ASP:HB3	2.01	0.42
2:E:157:LYS:NZ	8:E:2147:HOH:O	2.53	0.42
1:A:359:GLY:HA3	8:B:2088:HOH:O	2.20	0.41
1:B:563:HIS:HB2	8:B:2285:HOH:O	2.19	0.41
2:C:19:ILE:HD11	2:C:233:TYR:HA	2.02	0.41
3:D:63:VAL:HG13	3:D:174:VAL:HG23	2.02	0.41
1:B:542:ALA:HB3	1:B:543:PRO:HD3	2.02	0.41
1:A:139:MET:HE2	1:A:144:ILE:HG12	2.02	0.41
3:F:83:ILE:CD1	3:F:150:THR:HG21	2.49	0.41
1:A:718:MET:CG	8:A:2284:HOH:O	2.63	0.41
2:C:7:VAL:O	7:C:1236:AMP:C2	2.74	0.41
2:C:163:GLU:HA	2:C:169:LEU:HD23	2.03	0.41
1:A:295:LEU:HD12	1:A:295:LEU:C	2.46	0.41
1:A:77:ILE:HD12	1:A:77:ILE:HA	1.89	0.41
2:C:1:MET:HE3	8:C:2130:HOH:O	2.14	0.41
3:D:65:GLY:CA	8:D:2025:HOH:O	2.67	0.41
2:C:70:ASP:OD1	2:C:86:ARG:HD3	2.20	0.40
2:E:106:GLU:HB3	2:E:213:ILE:HB	2.04	0.40
2:E:157:LYS:CE	2:E:175:ASN:HD22	2.34	0.40
1:B:229:TYR:CG	8:B:2325:HOH:O	2.02	0.40
3:D:120:ILE:HB	3:D:131:THR:HB	2.04	0.40
1:B:515:LEU:HA	1:B:519:GLN:OE1	2.21	0.40
1:A:505:PRO:HD2	1:A:595:SER:O	2.21	0.40
1:B:72:ARG:HD2	1:B:355:TRP:CZ2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:OE2	2:E:156:ASN:OD1[4_545]	1.97	0.23
1:B:11:GLU:OE2	2:C:156:ASN:OD1[4_556]	2.05	0.15

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	727/729 (100%)	702 (97%)	25 (3%)	0	100	100
1	B	727/729 (100%)	700 (96%)	27 (4%)	0	100	100
2	C	229/264 (87%)	222 (97%)	4 (2%)	3 (1%)	9	5
2	E	234/264 (89%)	230 (98%)	4 (2%)	0	100	100
3	D	187/320 (58%)	179 (96%)	7 (4%)	1 (0%)	24	21
3	F	187/320 (58%)	184 (98%)	3 (2%)	0	100	100
All	All	2291/2626 (87%)	2217 (97%)	70 (3%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	56	ASP
2	C	157	LYS
3	D	31	SER
2	C	145	VAL

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	584/602 (97%)	573 (98%)	11 (2%)	50	56
1	B	578/602 (96%)	564 (98%)	14 (2%)	43	47
2	C	180/216 (83%)	169 (94%)	11 (6%)	17	14
2	E	177/216 (82%)	170 (96%)	7 (4%)	28	27
3	D	143/258 (55%)	133 (93%)	10 (7%)	14	10
3	F	150/258 (58%)	140 (93%)	10 (7%)	15	11
All	All	1812/2152 (84%)	1749 (96%)	63 (4%)	32	32

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	60	TYR
1	A	177	LEU
1	A	330	LEU
1	A	415	VAL
1	A	444	ARG
1	A	589	LEU
1	A	615	THR
1	A	650	LEU
1	A	667	LYS
1	A	718	MET
1	B	26	GLN
1	B	60	TYR
1	B	203	LEU
1	B	253	MET
1	B	441	SER
1	B	444	ARG
1	B	490	ARG
1	B	589	LEU
1	B	601	ARG
1	B	615	THR
1	B	621	VAL
1	B	650	LEU
1	B	667	LYS
1	B	718	MET
2	C	1	MET
2	C	32	MET
2	C	56	ASP

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Mol	Chain	Res	Type
2	C	89	ASP
2	C	96	ASP
2	C	120	VAL
2	C	156	ASN
2	C	157	LYS
2	C	160	ILE
2	C	203	LYS
2	C	231	ARG
3	D	21	LEU
3	D	37	VAL
3	D	60	LEU
3	D	71	ASP
3	D	91	VAL
3	D	105	SER
3	D	121	VAL
3	D	138	LYS
3	D	178	SER
3	D	180	GLN
2	E	1	MET
2	E	60	VAL
2	E	102	ARG
2	E	156	ASN
2	E	157	LYS
2	E	203	LYS
2	E	226	MET
3	F	29	LYS
3	F	37	VAL
3	F	49	VAL
3	F	60	LEU
3	F	64	LYS
3	F	66	SER
3	F	67	SER
3	F	83	ILE
3	F	91	VAL
3	F	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	GLN
1	A	535	ASN
1	A	563	HIS

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Mol	Chain	Res	Type
1	B	26	GLN
1	B	276	GLN
1	B	462	GLN
1	B	563	HIS
1	B	652	ASN
2	C	121	GLN
2	C	170	GLN
2	C	175	ASN
2	C	183	GLN
2	C	199	GLN
3	D	26	ASN
3	D	44	GLN
3	D	124	GLN
3	D	137	GLN
3	D	173	ASN
3	D	184	GLN
3	D	185	ASN
2	E	121	GLN
2	E	150	GLN
2	E	170	GLN
2	E	175	ASN
2	E	183	GLN
2	E	199	GLN
3	F	44	GLN
3	F	124	GLN
3	F	137	GLN
3	F	173	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
7	AMP	C	1236	-	25,25,25	1.27	4 (16%)	37,38,38	2.44	14 (37%)
6	SF4	A	1732	1	0,12,12	-	-	-	-	-
5	ADP	B	1731	-	28,29,29	1.27	5 (17%)	43,45,45	1.92	10 (23%)
5	ADP	A	1731	-	28,29,29	1.66	2 (7%)	43,45,45	1.74	8 (18%)
4	FMN	B	1730	1	33,33,33	1.49	7 (21%)	48,50,50	1.54	9 (18%)
7	AMP	E	1237	-	25,25,25	1.51	5 (20%)	37,38,38	2.46	15 (40%)
6	SF4	B	1732	1	0,12,12	-	-	-	-	-
4	FMN	A	1730	1	33,33,33	1.36	6 (18%)	48,50,50	1.59	10 (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
7	AMP	C	1236	-	-	4/10/26/26	0/3/3/3
6	SF4	A	1732	1	-	-	0/6/5/5
5	ADP	B	1731	-	-	2/16/32/32	0/3/3/3
5	ADP	A	1731	-	-	2/16/32/32	0/3/3/3
4	FMN	B	1730	1	-	1/18/18/18	0/3/3/3
7	AMP	E	1237	-	-	4/10/26/26	0/3/3/3
6	SF4	B	1732	1	-	-	0/6/5/5
4	FMN	A	1730	1	-	1/18/18/18	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1731	ADP	PA-O3A	7.18	1.67	1.59
7	E	1237	AMP	C2-N3	4.31	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1730	FMN	C4A-N5	3.25	1.37	1.30
7	C	1236	AMP	C2-N3	3.21	1.39	1.33
7	E	1237	AMP	C2-N1	3.09	1.39	1.33
5	A	1731	ADP	C2-N3	3.02	1.39	1.33
5	B	1731	ADP	C8-N7	2.95	1.37	1.31
4	B	1730	FMN	C9A-N10	-2.83	1.36	1.41
5	B	1731	ADP	C5-N7	-2.79	1.34	1.39
7	C	1236	AMP	C2-N1	2.78	1.38	1.33
4	B	1730	FMN	C1'-C2'	2.68	1.56	1.52
4	A	1730	FMN	C10-N1	2.58	1.38	1.33
4	B	1730	FMN	C9-C8	-2.50	1.36	1.39
4	A	1730	FMN	C9-C8	-2.44	1.36	1.39
5	B	1731	ADP	C2-N3	2.42	1.38	1.33
7	E	1237	AMP	O4'-C4'	-2.42	1.39	1.45
7	C	1236	AMP	C8-N7	2.40	1.36	1.31
7	E	1237	AMP	O5'-C5'	-2.39	1.35	1.44
7	E	1237	AMP	C8-N7	2.38	1.36	1.31
7	C	1236	AMP	O5'-C5'	-2.38	1.35	1.44
4	B	1730	FMN	C4A-N5	2.31	1.35	1.30
4	B	1730	FMN	C5'-C4'	2.30	1.54	1.51
4	A	1730	FMN	C1'-N10	2.22	1.53	1.47
5	B	1731	ADP	C2-N1	2.19	1.37	1.33
4	A	1730	FMN	C6-C5A	-2.16	1.36	1.40
4	A	1730	FMN	C6-C7	2.13	1.42	1.39
4	B	1730	FMN	C6-C5A	-2.08	1.36	1.40
4	B	1730	FMN	P-O2P	-2.06	1.47	1.54
5	B	1731	ADP	PA-O2A	-2.02	1.46	1.55

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1236	AMP	N3-C2-N1	-6.80	118.29	128.58
7	C	1236	AMP	O2P-P-O5'	6.56	123.76	106.67
7	E	1237	AMP	N3-C2-N1	-6.36	118.96	128.58
5	B	1731	ADP	N9-C8-N7	-5.44	106.22	113.94
7	E	1237	AMP	O2P-P-O5'	5.22	120.29	106.67
5	A	1731	ADP	N3-C2-N1	-5.05	120.94	128.58
5	B	1731	ADP	N3-C2-N1	-5.04	120.95	128.58
7	C	1236	AMP	C5-C4-N3	-4.49	120.53	126.72
7	E	1237	AMP	O5'-P-O1P	-4.43	94.48	106.44
7	E	1237	AMP	N9-C8-N7	-4.37	107.74	113.94
7	E	1237	AMP	C5-N7-C8	4.26	110.14	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1731	ADP	N9-C8-N7	-4.20	107.98	113.94
7	E	1237	AMP	C4-C5-N7	-4.20	105.78	110.58
5	B	1731	ADP	C5-C4-N3	-4.18	120.97	126.72
5	B	1731	ADP	C5-N7-C8	4.16	109.98	103.45
7	C	1236	AMP	O5'-P-O1P	-4.11	95.33	106.44
5	A	1731	ADP	C5-N7-C8	3.87	109.53	103.45
7	E	1237	AMP	C5-C4-N3	-3.62	121.73	126.72
4	A	1730	FMN	C9A-C5A-N5	-3.60	118.64	122.45
7	C	1236	AMP	C2-N3-C4	3.59	120.60	111.83
5	A	1731	ADP	C4-C5-N7	-3.54	106.53	110.58
4	B	1730	FMN	C10-C4A-N5	-3.36	117.95	124.81
4	A	1730	FMN	C6-C5A-N5	3.35	124.01	118.44
5	A	1731	ADP	C5-C4-N3	-3.30	122.18	126.72
7	C	1236	AMP	C5-N7-C8	3.26	108.58	103.45
5	B	1731	ADP	C2-N3-C4	3.22	119.69	111.83
4	B	1730	FMN	C4A-C10-N10	3.11	120.93	116.48
4	B	1730	FMN	C6-C5A-N5	3.10	123.59	118.44
7	C	1236	AMP	C4-C5-N7	-3.10	107.04	110.58
5	A	1731	ADP	O2A-PA-O3A	3.09	115.62	107.27
5	A	1731	ADP	C2-N3-C4	3.07	119.32	111.83
4	A	1730	FMN	C8M-C8-C9	-3.07	114.17	119.57
4	A	1730	FMN	O4-C4-C4A	-3.01	118.60	126.53
7	C	1236	AMP	N9-C8-N7	-2.98	109.71	113.94
7	E	1237	AMP	C2-N3-C4	2.93	118.98	111.83
4	A	1730	FMN	C5A-C9A-N10	2.88	120.57	117.97
4	B	1730	FMN	C9A-C5A-N5	-2.85	119.43	122.45
5	B	1731	ADP	O2A-PA-O3A	2.79	114.82	107.27
5	B	1731	ADP	O3B-PB-O3A	2.73	113.78	104.64
4	B	1730	FMN	O4-C4-C4A	-2.71	119.39	126.53
7	C	1236	AMP	C2-N1-C6	2.64	123.07	118.73
4	A	1730	FMN	C4A-C10-N10	2.63	120.25	116.48
7	E	1237	AMP	C2'-C3'-C4'	-2.60	97.59	102.61
7	E	1237	AMP	C5'-C4'-C3'	2.56	124.44	115.21
7	E	1237	AMP	C2-N1-C6	2.55	122.92	118.73
4	B	1730	FMN	C7M-C7-C8	-2.53	115.59	120.76
7	C	1236	AMP	C2'-C1'-N9	-2.45	107.22	113.30
7	C	1236	AMP	N3-C4-N9	2.45	131.33	127.17
7	E	1237	AMP	O2'-C2'-C1'	-2.43	101.74	110.10
5	B	1731	ADP	N3-C4-N9	2.42	131.29	127.17
7	E	1237	AMP	C4-N9-C8	2.38	108.24	105.74
4	A	1730	FMN	C9A-C9-C8	2.36	123.97	119.22
4	A	1730	FMN	C1'-C2'-C3'	2.36	116.05	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1730	FMN	C7M-C7-C8	-2.35	115.96	120.76
4	A	1730	FMN	C10-C4A-N5	-2.31	120.09	124.81
5	B	1731	ADP	C4-C5-N7	-2.28	107.97	110.58
4	B	1730	FMN	C4-C4A-C10	2.24	120.78	116.93
7	C	1236	AMP	C5'-C4'-C3'	2.23	123.26	115.21
4	B	1730	FMN	C4-C4A-N5	2.21	121.26	118.21
5	B	1731	ADP	C4-N9-C8	2.21	108.06	105.74
5	A	1731	ADP	C4-N9-C8	2.17	108.02	105.74
7	C	1236	AMP	C5-C4-N9	2.12	108.12	105.81
7	C	1236	AMP	O2'-C2'-C1'	-2.09	102.91	110.10
7	E	1237	AMP	C5-C4-N9	2.08	108.08	105.81
4	B	1730	FMN	C5A-N5-C4A	2.08	121.45	118.09
7	E	1237	AMP	C6-C5-C4	2.03	119.95	117.18

There are no chirality outliers.

All (14) torsion outliers are listed below:

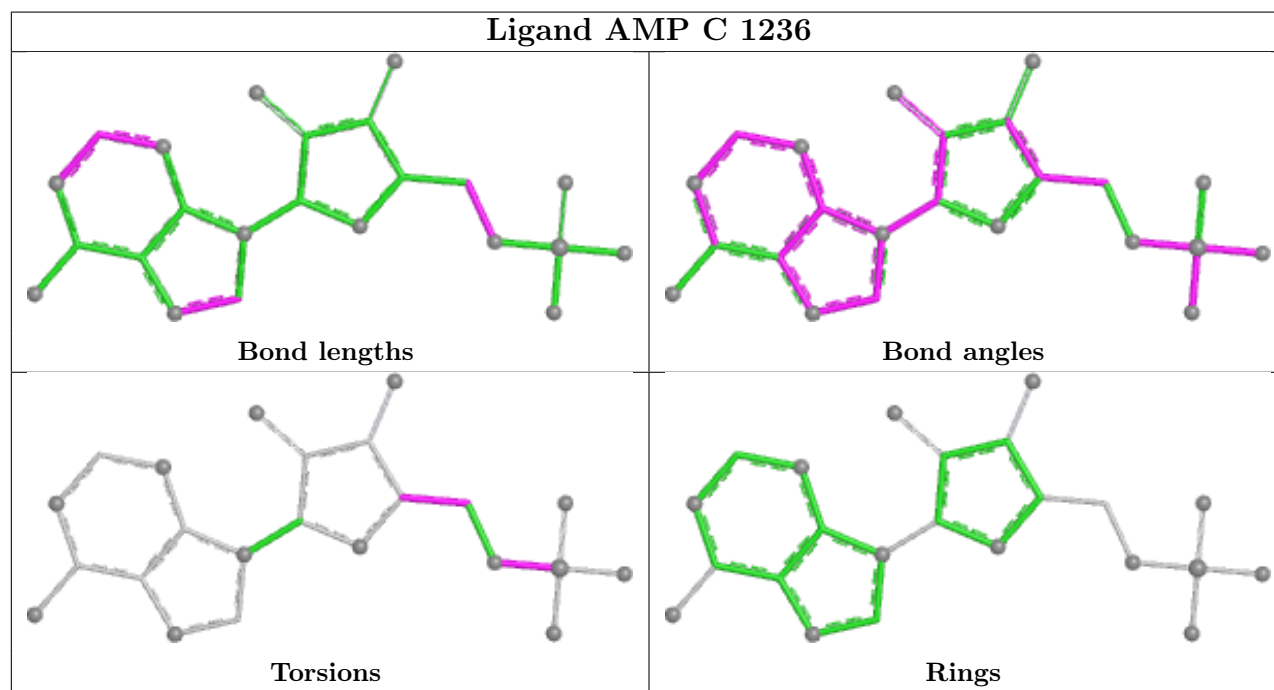
Mol	Chain	Res	Type	Atoms
7	C	1236	AMP	C5'-O5'-P-O2P
7	C	1236	AMP	C5'-O5'-P-O3P
7	E	1237	AMP	C5'-O5'-P-O3P
7	C	1236	AMP	C5'-O5'-P-O1P
7	E	1237	AMP	C5'-O5'-P-O1P
7	E	1237	AMP	C3'-C4'-C5'-O5'
7	E	1237	AMP	C5'-O5'-P-O2P
5	B	1731	ADP	PB-O3A-PA-O2A
4	A	1730	FMN	C4'-C5'-O5'-P
4	B	1730	FMN	C4'-C5'-O5'-P
5	A	1731	ADP	PB-O3A-PA-O2A
5	A	1731	ADP	PB-O3A-PA-O1A
5	B	1731	ADP	PB-O3A-PA-O1A
7	C	1236	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

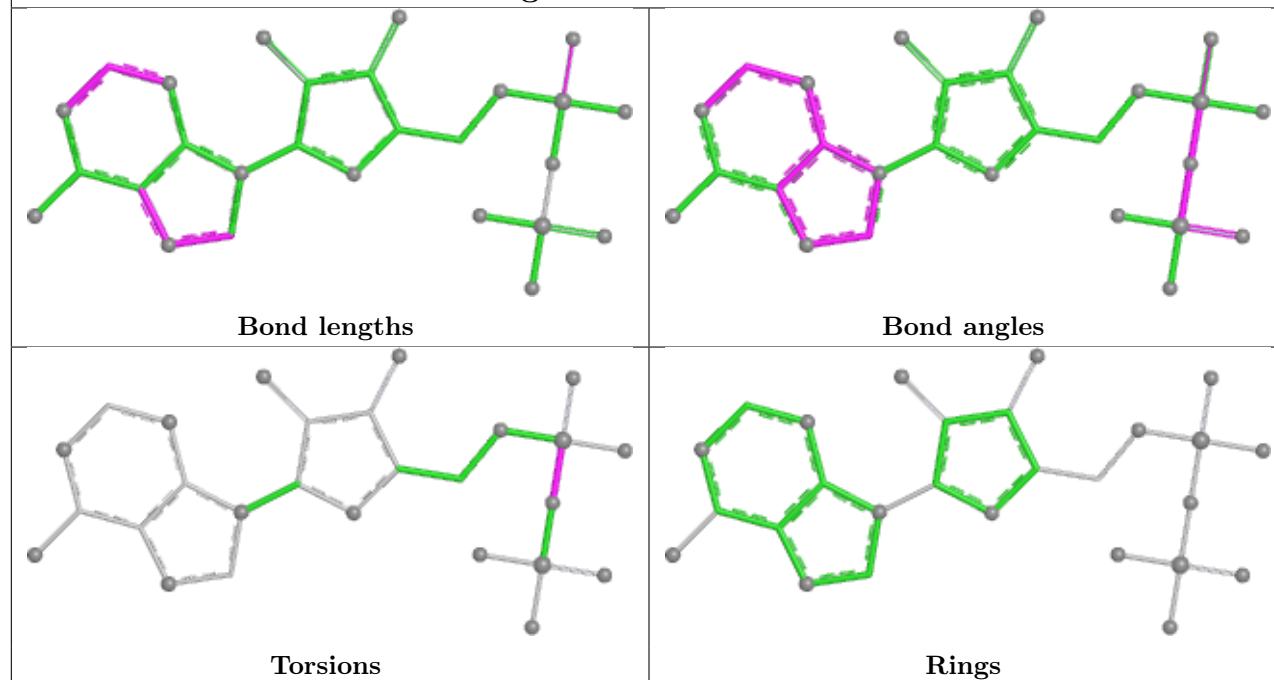
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1236	AMP	2	0
4	B	1730	FMN	1	0
7	E	1237	AMP	1	0
6	B	1732	SF4	2	0

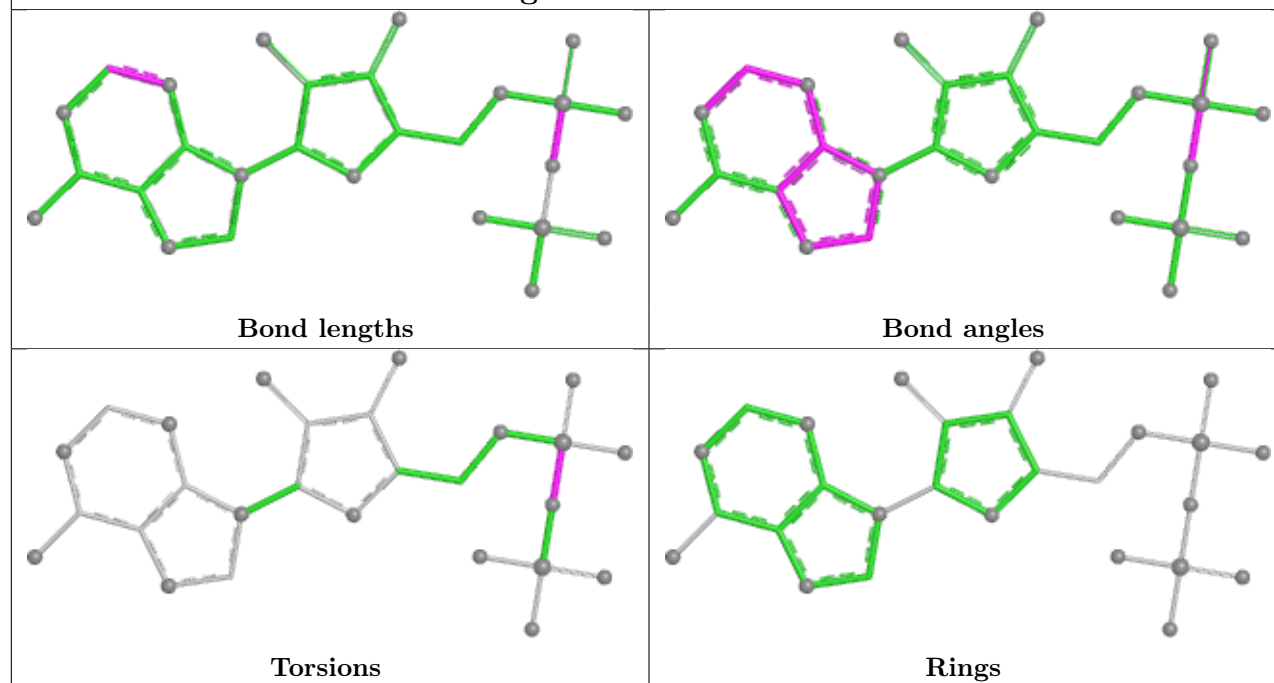
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

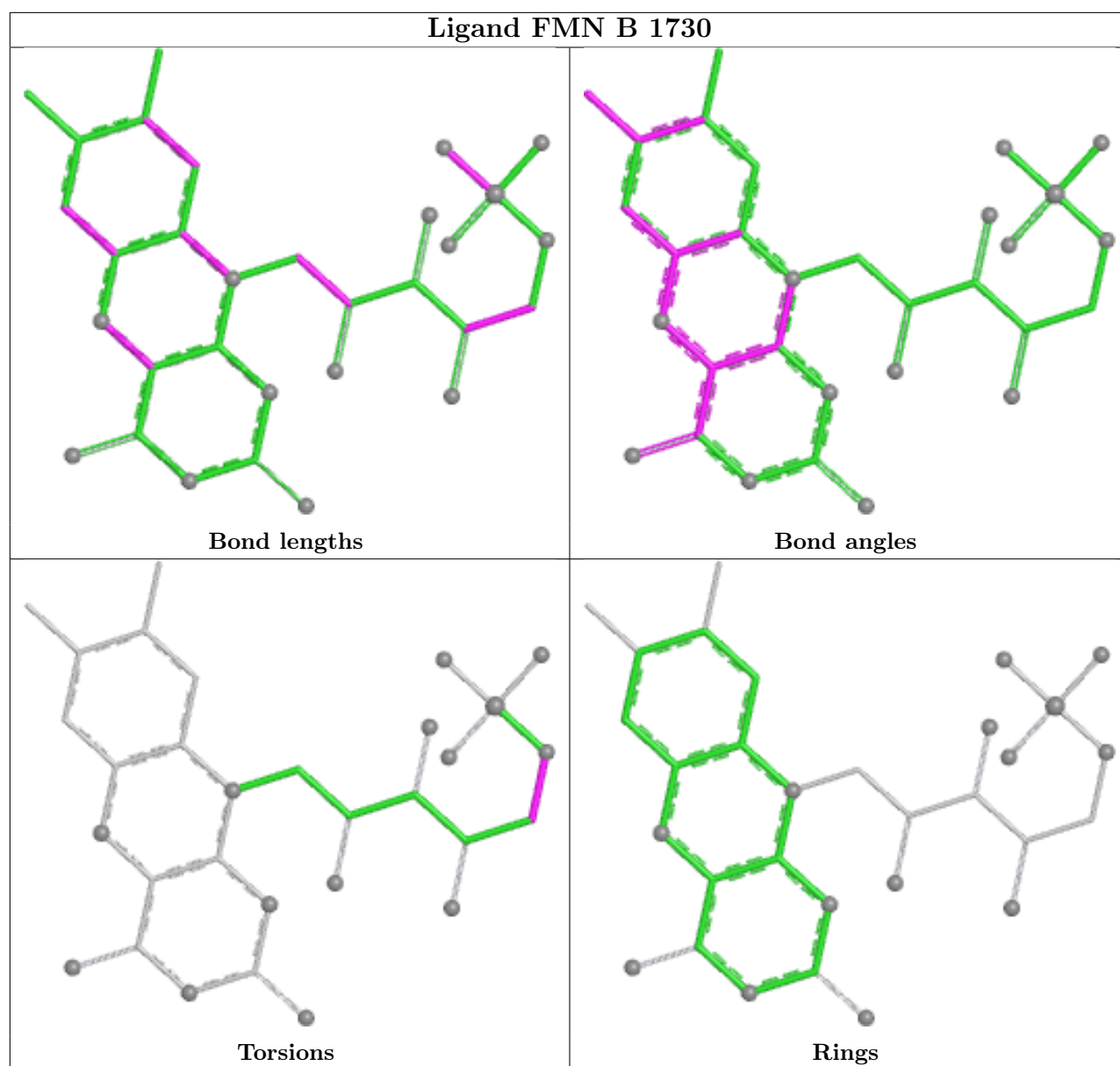


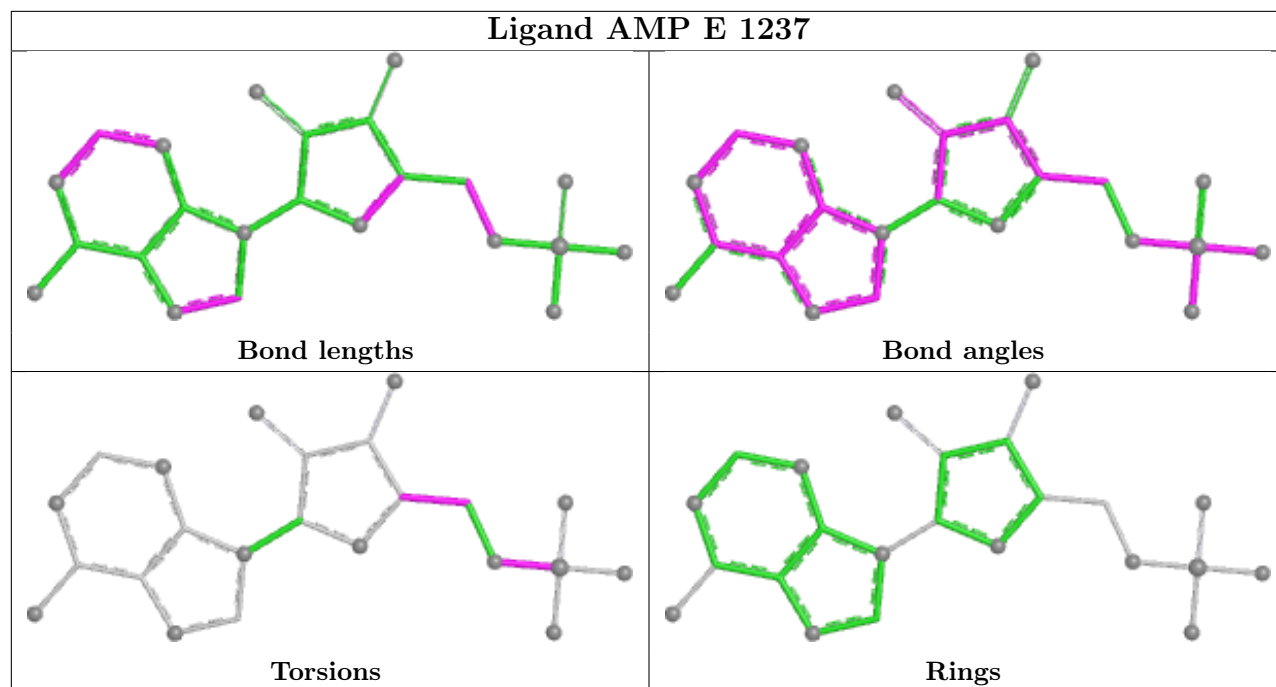
Ligand ADP B 1731

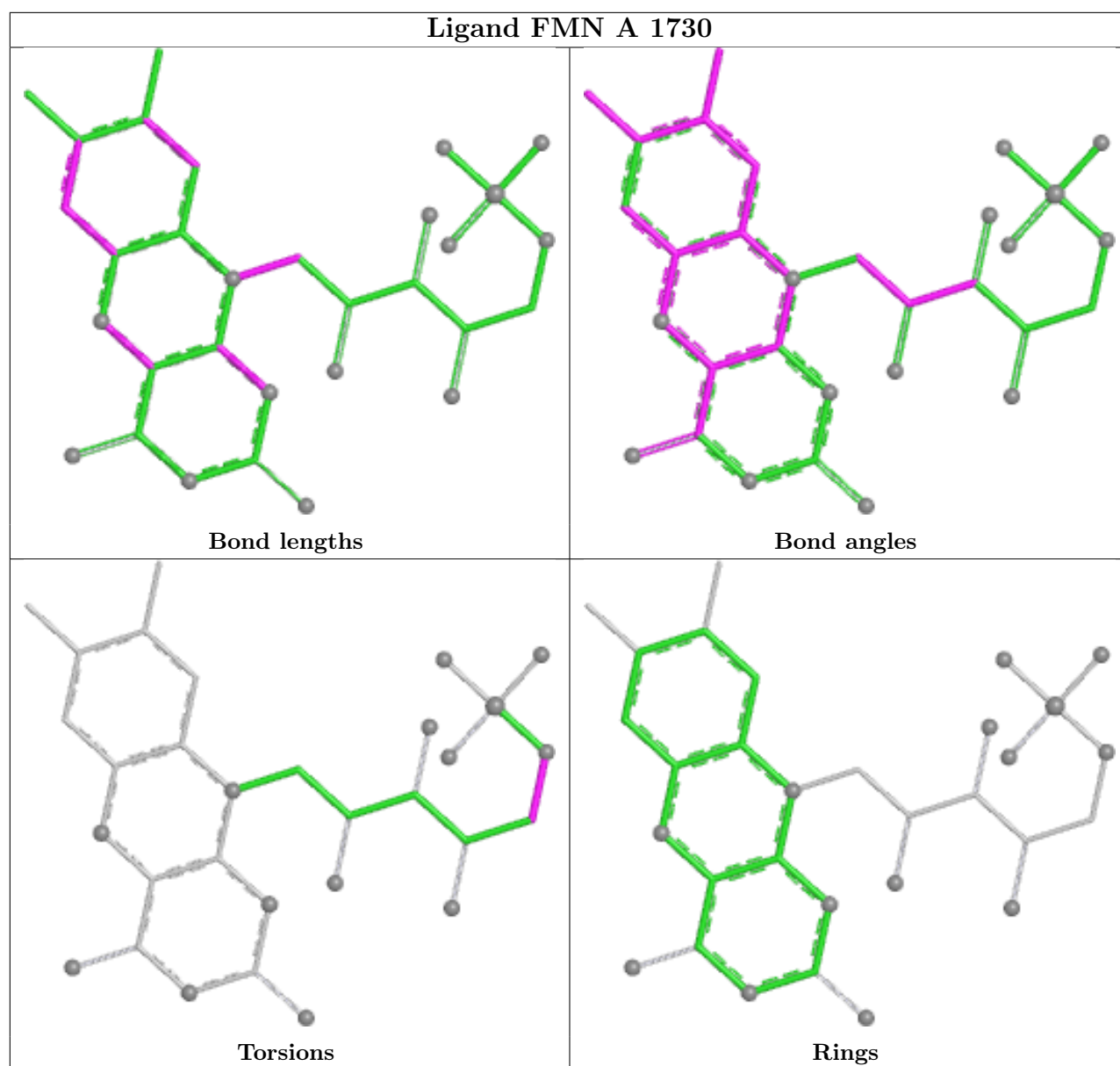


Ligand ADP A 1731









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	729/729 (100%)	-0.44	2 (0%) 90 89	21, 28, 40, 47	0
1	B	729/729 (100%)	-0.53	4 (0%) 87 87	18, 26, 38, 53	0
2	C	233/264 (88%)	0.04	3 (1%) 75 74	25, 35, 56, 66	0
2	E	236/264 (89%)	-0.01	7 (2%) 52 51	25, 33, 50, 58	0
3	D	189/320 (59%)	0.68	20 (10%) 11 10	32, 50, 66, 76	0
3	F	189/320 (59%)	0.02	3 (1%) 70 70	27, 36, 52, 63	0
All	All	2305/2626 (87%)	-0.25	39 (1%) 69 68	18, 30, 53, 76	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	22	ASP	4.1
3	D	174	VAL	3.5
2	E	54	ASP	3.4
2	E	23	GLY	3.4
3	F	32	GLY	3.2
3	D	177	PRO	3.0
3	D	31	SER	2.9
2	E	16	ASP	2.9
3	D	170	VAL	2.9
3	D	66	SER	2.9
3	D	176	ALA	2.8
2	C	156	ASN	2.7
2	E	24	MET	2.7
3	D	32	GLY	2.6
3	D	147	GLY	2.6
1	A	24	PHE	2.6
3	D	33	GLU	2.5
3	D	179	VAL	2.5
2	E	217	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	126	ASP	2.4
3	D	65	GLY	2.3
3	D	180	GLN	2.3
1	B	11	GLU	2.3
1	B	563	HIS	2.3
3	D	149	SER	2.2
3	D	171	VAL	2.2
3	F	180	GLN	2.2
1	B	458	ASN	2.2
3	D	62	VAL	2.2
3	D	87	ASN	2.2
2	C	22	ASP	2.2
2	C	54	ASP	2.2
2	E	55	THR	2.1
1	A	632	TRP	2.1
1	B	601	ARG	2.1
3	D	44	GLN	2.1
3	F	31	SER	2.1
3	D	178	SER	2.0
3	D	30	LYS	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($\text{\AA}^2$)	Q<0.9
6	SF4	B	1732	8/8	0.89	0.15	28,29,43,49	0
4	FMN	B	1730	31/31	0.96	0.07	19,23,26,28	0
4	FMN	A	1730	31/31	0.96	0.07	18,23,25,27	0

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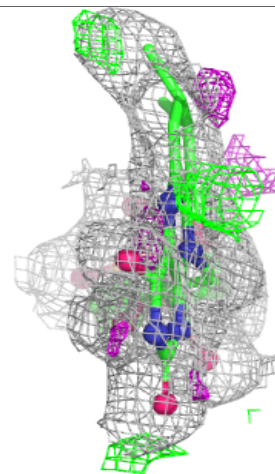
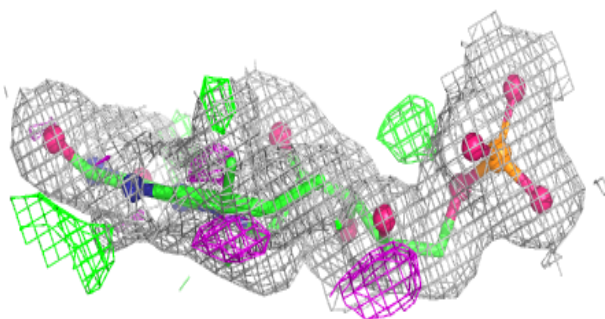
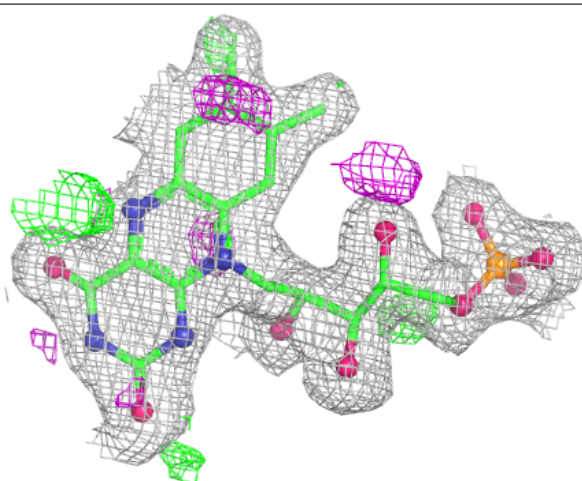
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	AMP	C	1236	23/23	0.96	0.06	26,30,37,38	0
7	AMP	E	1237	23/23	0.97	0.07	23,28,33,35	0
5	ADP	A	1731	27/27	0.99	0.04	23,28,30,31	0
5	ADP	B	1731	27/27	0.99	0.04	20,24,28,29	0
6	SF4	A	1732	8/8	0.99	0.07	29,31,32,36	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.

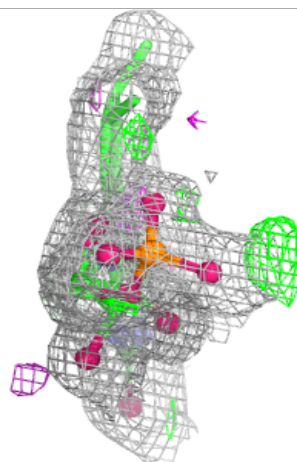
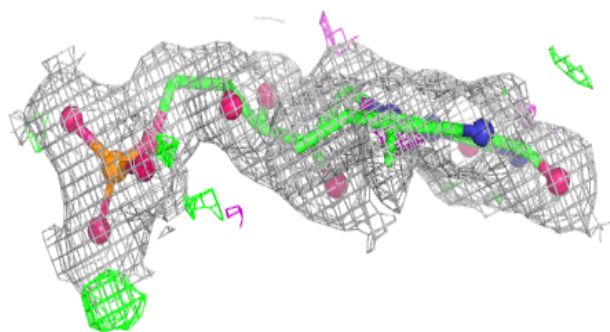
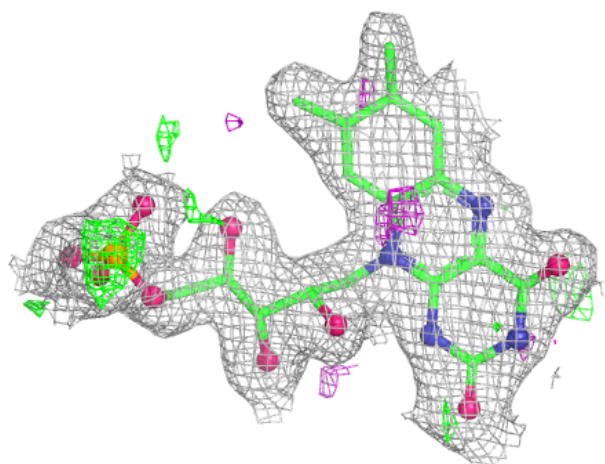
Electron density around FMN B 1730:

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



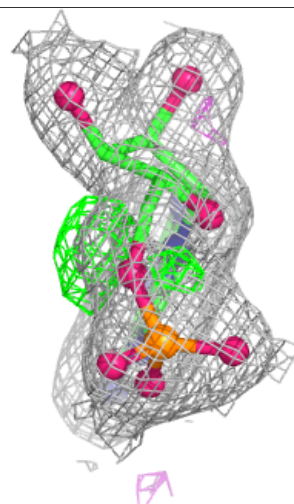
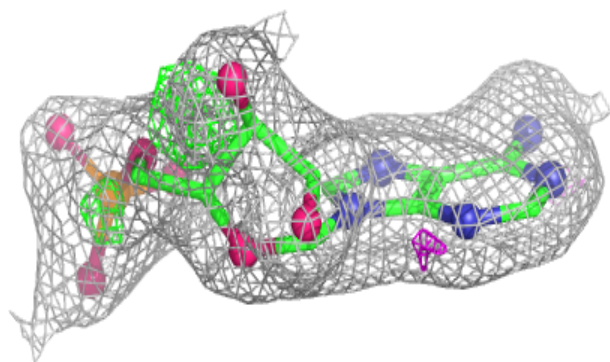
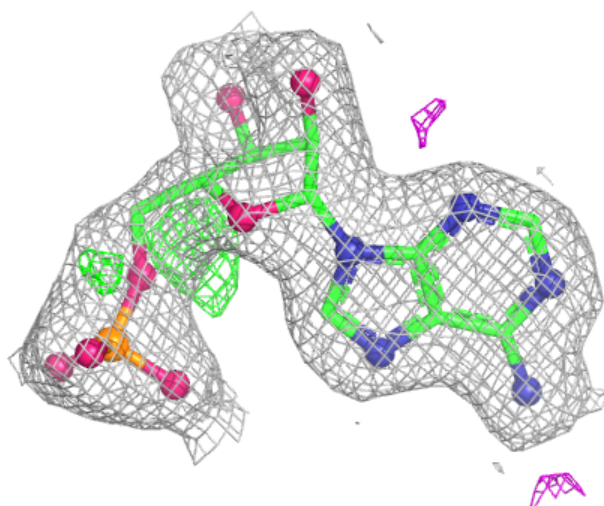
Electron density around FMN A 1730:

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



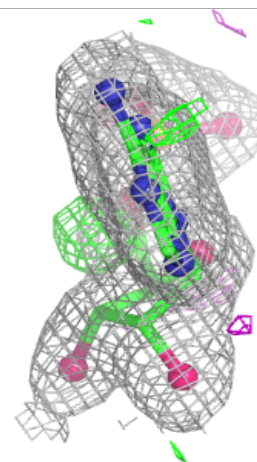
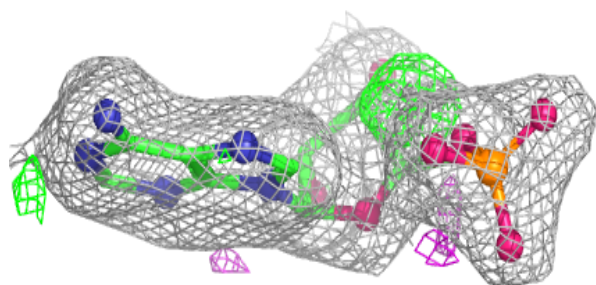
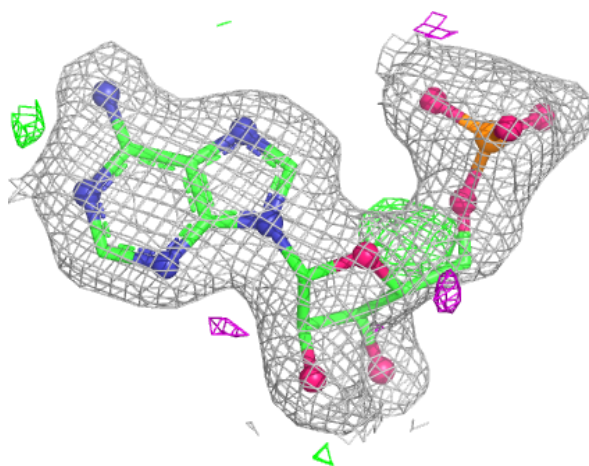
Electron density around AMP C 1236:

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



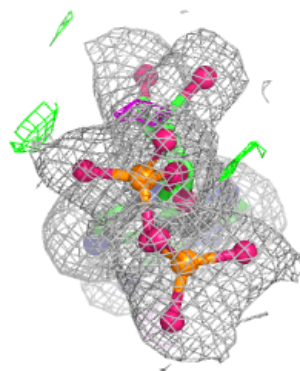
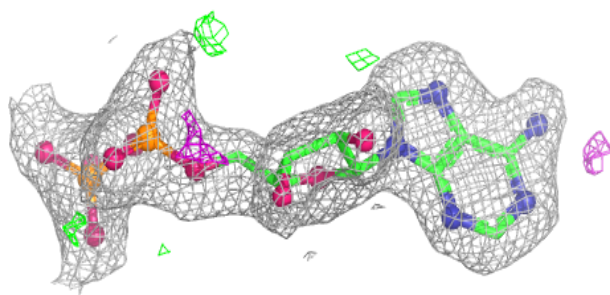
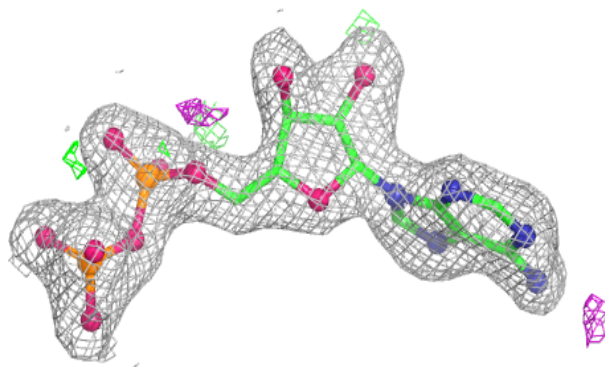
Electron density around AMP E 1237:

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

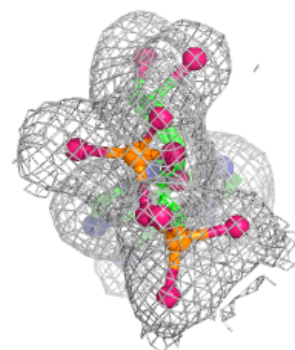
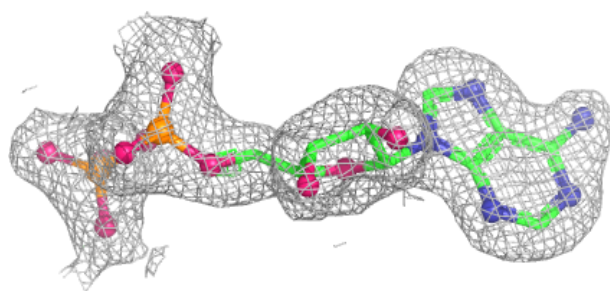
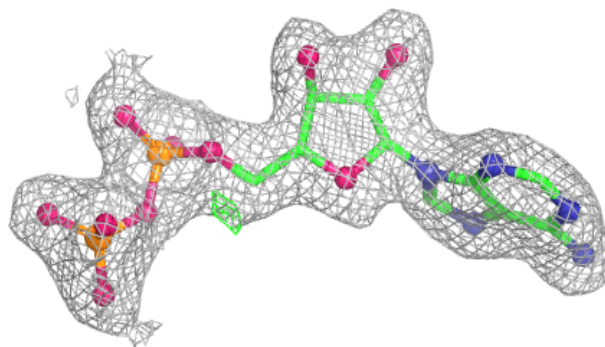


Electron density around ADP A 1731:

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

**Electron density around ADP B 1731:**

$2mF_o-DF_c$ (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.