



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2023 – 12:13 am GMT

PDB ID : 1O94  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

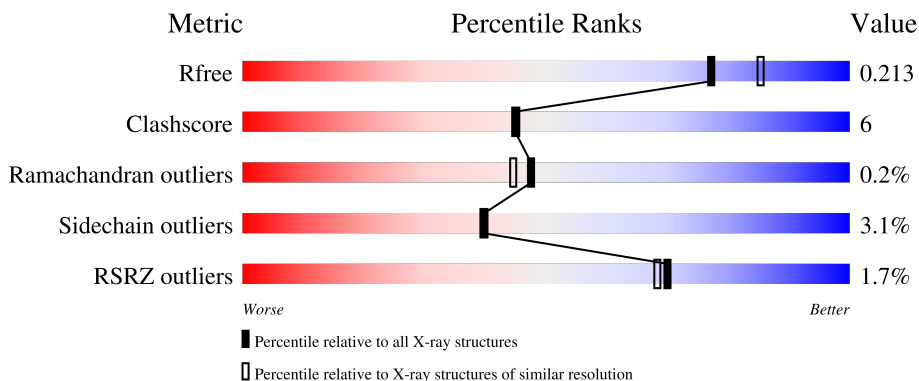
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



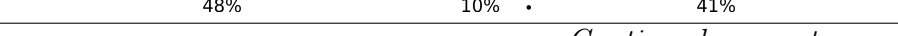
The reported resolution of this entry is 2.00 Å.

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.



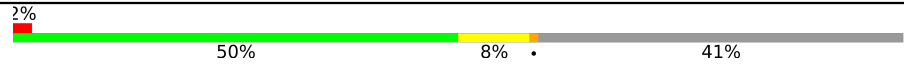
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	 87% 11% .
2	C	264	 % 68% 16% . . 12%
2	E	264	 2% 73% 12% 5% 11%
3	D	320	 7% 48% 10% . 41%

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Mol	Chain	Length	Quality of chain
3	F	320	

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
			Total	C	N	O	S			
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			

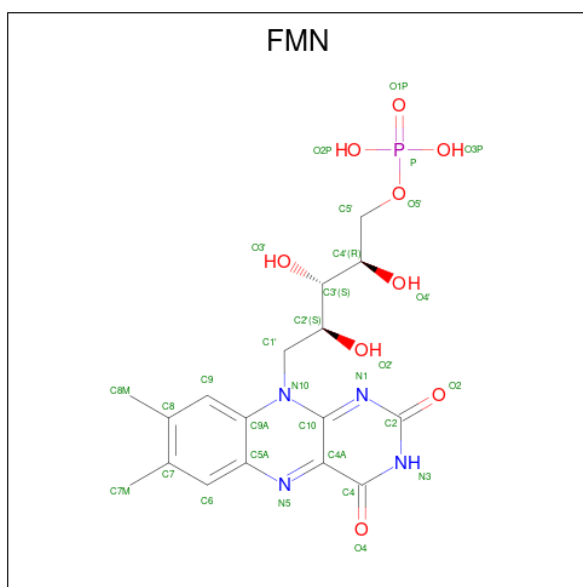
- Molecule 2 is a protein called ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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.

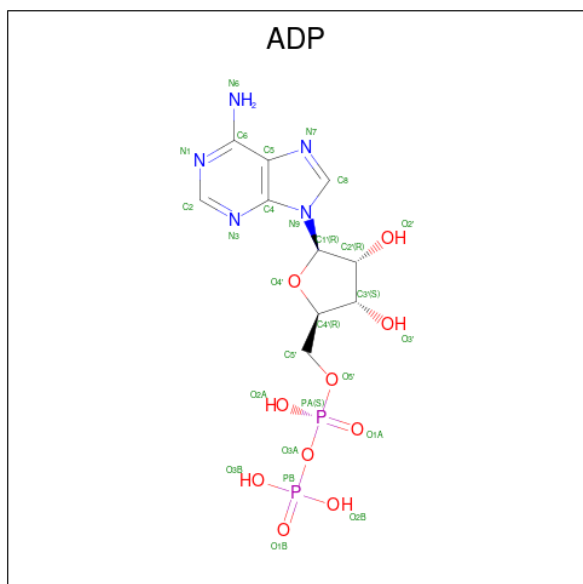
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	189	Total	C	N	O	0	0	0
			1354	857	230	267			
3	F	189	Total	C	N	O	0	0	0
			1376	870	232	274			

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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 (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



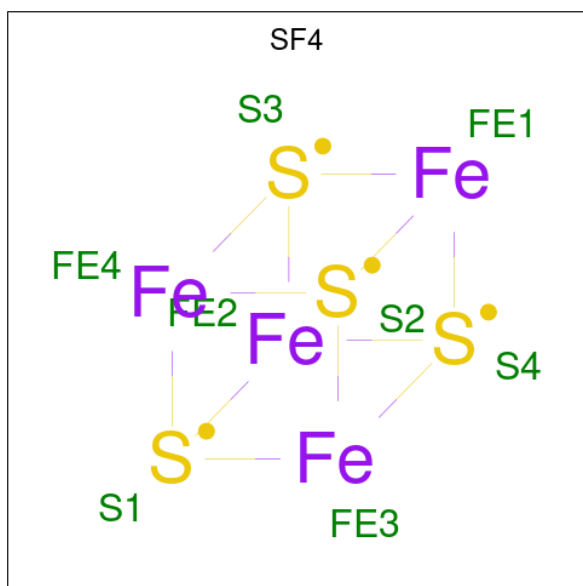
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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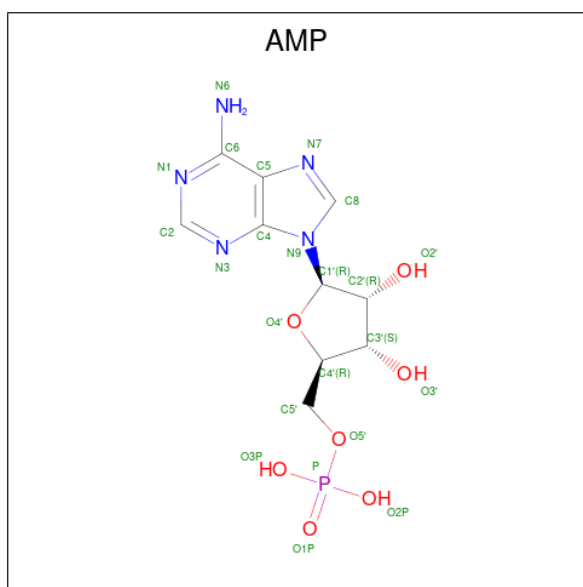
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
5	B	1	27	10	5	10	2	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



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

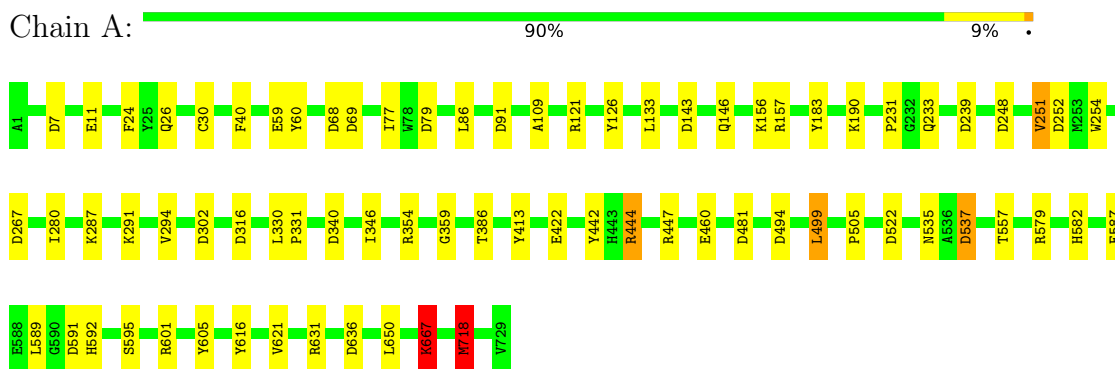
- Molecule 8 is water.

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		

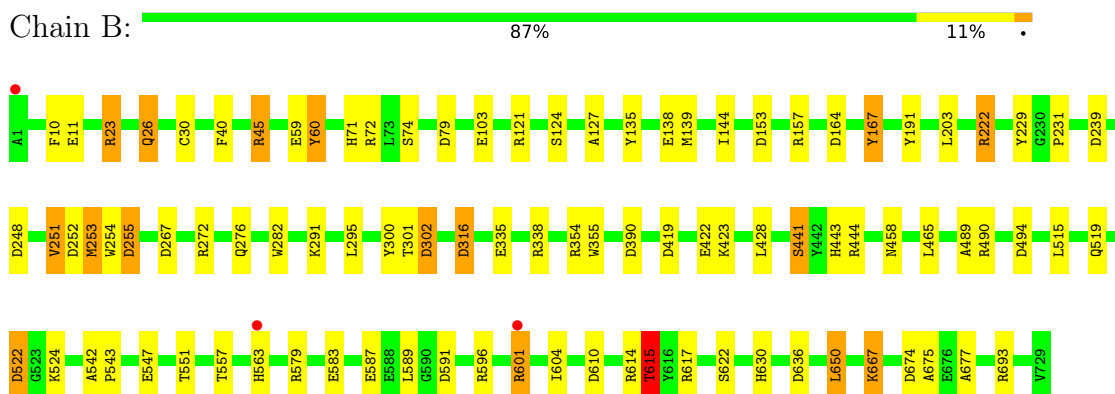
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

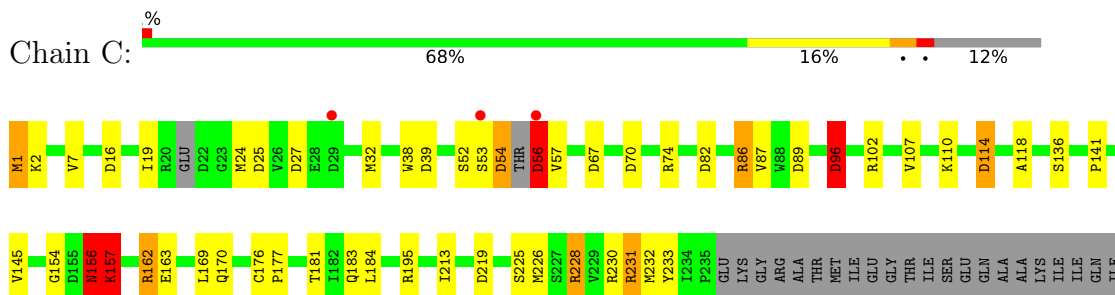
- Molecule 1: TRIMETHYLAMINE DEHYDROGENASE



- Molecule 1: TRIMETHYLAMINE DEHYDROGENASE



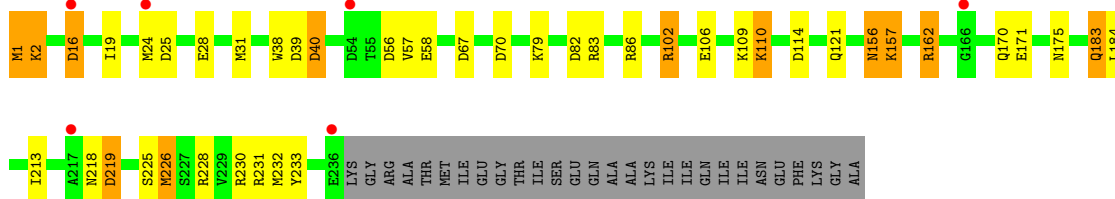
- Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT



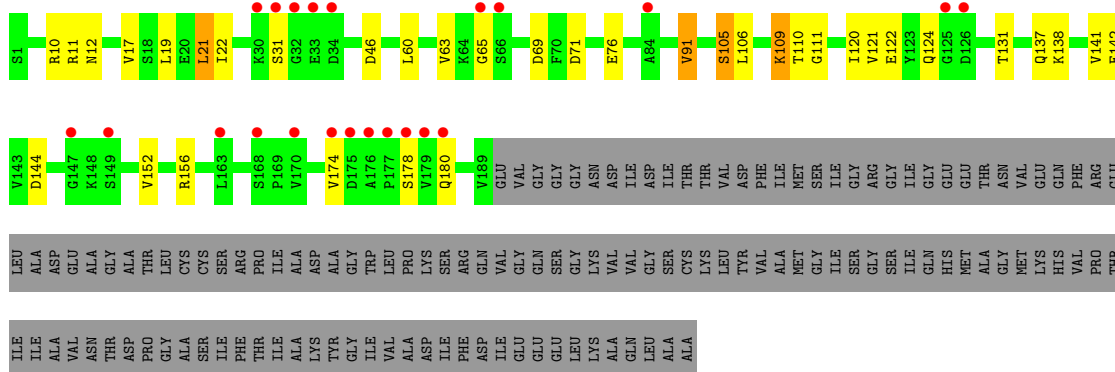


ILE  
ASN  
GLU  
PHE  
LYS  
GLY  
ALA

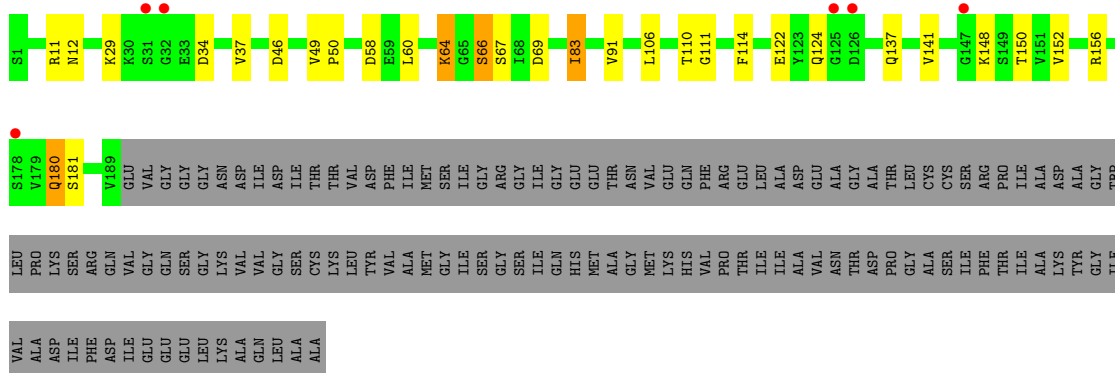
• Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT



• Molecule 3: ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT



• Molecule 3: ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.93Å 211.54Å 125.97Å 90.00° 100.03° 90.00°	Depositor
Resolution (Å)	19.88 – 2.00 19.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.88-2.00) 94.8 (19.90-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.1.08	Depositor
R, $R_{free}$	0.172 , 0.212 0.175 , 0.213	Depositor DCC
$R_{free}$ test set	9811 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtrriage
Anisotropy	0.550	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19925	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ADP, AMP, FMN, SF4

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	1.04	1/5834 (0.0%)	1.02	29/7918 (0.4%)
1	B	1.11	8/5818 (0.1%)	1.03	31/7902 (0.4%)
2	C	1.06	2/1772 (0.1%)	1.12	18/2402 (0.7%)
2	E	0.97	1/1775 (0.1%)	1.21	18/2408 (0.7%)
3	D	0.72	0/1378	0.90	4/1884 (0.2%)
3	F	0.87	0/1400	0.97	6/1913 (0.3%)
All	All	1.03	12/17977 (0.1%)	1.04	106/24427 (0.4%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	54	ASP	C-N	21.72	1.83	1.34
1	B	601	ARG	CG-CD	8.79	1.74	1.51
2	E	110	LYS	CE-NZ	8.01	1.69	1.49
2	C	110	LYS	CE-NZ	7.27	1.67	1.49
1	A	251	VAL	CB-CG2	-6.27	1.39	1.52
1	B	291	LYS	CD-CE	6.08	1.66	1.51
1	B	675	ALA	CA-CB	5.81	1.64	1.52
1	B	596	ARG	CG-CD	5.72	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	677	ALA	CA-CB	5.38	1.63	1.52
1	B	191	TYR	CD1-CE1	5.35	1.47	1.39
1	B	601	ARG	NE-CZ	5.13	1.39	1.33
1	B	251	VAL	CB-CG2	-5.09	1.42	1.52

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	162	ARG	NE-CZ-NH2	-16.61	112.00	120.30
2	E	162	ARG	NE-CZ-NH1	14.90	127.75	120.30
1	A	157	ARG	NE-CZ-NH1	-14.87	112.86	120.30
2	E	86	ARG	NE-CZ-NH2	-13.81	113.39	120.30
2	C	54	ASP	C-N-CA	13.74	156.06	121.70
2	C	86	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	A	157	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	A	354	ARG	NE-CZ-NH1	-9.11	115.74	120.30
2	C	16	ASP	CB-CG-OD2	8.89	126.30	118.30
3	D	46	ASP	CB-CG-OD2	7.85	125.37	118.30
1	B	239	ASP	CB-CG-OD2	7.67	125.20	118.30
1	B	157	ARG	NE-CZ-NH1	-7.56	116.52	120.30
2	E	16	ASP	N-CA-C	-7.37	91.12	111.00
1	A	636	ASP	CB-CG-OD2	7.26	124.83	118.30
1	B	302	ASP	CB-CG-OD2	7.18	124.77	118.30
1	A	537	ASP	CB-CG-OD2	7.08	124.67	118.30
1	B	272	ARG	NE-CZ-NH2	-6.99	116.80	120.30
2	E	219	ASP	CB-CG-OD2	6.92	124.52	118.30
1	A	7	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	267	ASP	CB-CG-OD2	6.86	124.47	118.30
2	C	74	ARG	CG-CD-NE	-6.85	97.41	111.80
1	B	164	ASP	CB-CG-OD2	6.76	124.39	118.30
2	E	231	ARG	CB-CA-C	-6.76	96.89	110.40
1	B	636	ASP	CB-CG-OD2	6.59	124.23	118.30
3	F	106	LEU	CA-CB-CG	6.57	130.40	115.30
1	B	79	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	252	ASP	CB-CG-OD2	6.46	124.12	118.30
2	E	86	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	79	ASP	CB-CG-OD1	6.43	124.09	118.30
1	B	650	LEU	CB-CG-CD2	6.40	121.89	111.00
2	E	86	ARG	CG-CD-NE	-6.39	98.39	111.80
1	B	591	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	23	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	287	LYS	CD-CE-NZ	-6.24	97.35	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ARG	NE-CZ-NH1	-6.21	117.19	120.30
2	E	82	ASP	CB-CG-OD2	6.15	123.84	118.30
2	E	110	LYS	CD-CE-NZ	6.14	125.81	111.70
3	F	122	GLU	CB-CA-C	-6.11	98.18	110.40
3	D	69	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	316	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	69	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	481	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	522	ASP	CB-CG-OD2	5.99	123.69	118.30
2	C	39	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	615	THR	CB-CA-C	-5.96	95.52	111.60
2	C	219	ASP	CB-CG-OD2	5.93	123.63	118.30
1	B	390	ASP	CB-CG-OD2	5.90	123.61	118.30
2	C	82	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	68	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	447	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	E	39	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	153	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	338	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	316	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	494	ASP	CB-CG-OD2	5.78	123.50	118.30
2	E	40	ASP	CB-CG-OD2	5.77	123.50	118.30
2	E	56	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	340	ASP	CB-CG-OD2	5.71	123.44	118.30
2	C	156	ASN	N-CA-C	5.70	126.38	111.00
2	E	70	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	614	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	143	ASP	CB-CG-OD1	5.62	123.36	118.30
3	D	106	LEU	CA-CB-CG	5.60	128.18	115.30
2	E	114	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	610	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	650	LEU	CA-CB-CG	5.52	128.00	115.30
2	C	157	LYS	N-CA-CB	5.52	120.54	110.60
2	C	16	ASP	N-CA-C	-5.52	96.10	111.00
1	A	444	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	C	162	ARG	CG-CD-NE	5.47	123.30	111.80
3	F	46	ASP	CB-CG-OD2	5.47	123.22	118.30
2	C	86	ARG	CG-CD-NE	-5.43	100.40	111.80
3	D	10	ARG	NE-CZ-NH2	-5.42	117.59	120.30
3	F	34	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	667	LYS	CD-CE-NZ	-5.42	99.24	111.70
1	A	718	MET	CG-SD-CE	5.41	108.86	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	91	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	231	PRO	C-N-CA	-5.36	111.05	122.30
1	B	267	ASP	CB-CG-OD2	5.35	123.12	118.30
2	C	114	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	522	ASP	CB-CG-OD2	5.31	123.08	118.30
2	C	2	LYS	CB-CG-CD	-5.29	97.85	111.60
2	C	86	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	499	LEU	CB-CG-CD2	-5.21	102.14	111.00
2	C	27	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	239	ASP	CB-CG-OD2	5.17	122.96	118.30
3	F	69	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	255	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	591	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	579	ARG	NE-CZ-NH1	-5.13	117.74	120.30
2	C	96	ASP	CB-CA-C	5.13	120.65	110.40
1	B	419	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	441	SER	CB-CA-C	-5.11	100.39	110.10
1	A	252	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	23	ARG	CG-CD-NE	-5.08	101.14	111.80
1	B	222	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	494	ASP	CB-CG-OD2	5.08	122.87	118.30
2	E	2	LYS	CB-CG-CD	-5.06	98.44	111.60
2	E	67	ASP	CB-CG-OD2	5.05	122.85	118.30
3	F	58	ASP	CB-CG-OD2	5.05	122.84	118.30
2	E	109	LYS	CD-CE-NZ	5.04	123.29	111.70
1	A	248	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	693	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	C	67	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	302	ASP	CB-CG-OD2	5.00	122.80	118.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5692	0	5444	43	1
1	B	5676	0	5423	60	1
2	C	1749	0	1722	48	1
2	E	1751	0	1716	45	1
3	D	1354	0	1311	28	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
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	9	0
8	D	73	0	0	2	0
8	E	198	0	0	14	0
8	F	151	0	0	3	0
All	All	19925	0	17058	225	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 6.

All (225) 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	1.30
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:ASP:HA	2:E:232:MET:HE3	1.18	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
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:C:25:ASP:HA	2:C:232:MET:HE3	1.49	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:E:25:ASP:CA	2:E:232:MET:HE3	2.02	0.85
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:231:ARG:HH12	3:D:142:GLU:CD	2.02	0.64
1:B:615:THR:CB	8:B:2680:HOH:O	2.32	0.63
2:E:218:ASN:C	8:E:2191:HOH:O	2.35	0.63
1:B:276:GLN:HE22	1:B:302:ASP:H	1.46	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: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
1:A:156:LYS:CE	8:A:2172:HOH:O	2.48	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
1:B:667:LYS:HD2	8:B:2738:HOH:O	2.02	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: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:A:718:MET:HE3	8:A:2284:HOH:O	2.07	0.55
1:B:276:GLN:NE2	1:B:301:THR:H	2.05	0.55
2:E:1:MET:HG3	2:E:2:LYS:N	2.22	0.55
2:E:1:MET:HE3	8:E:2116:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:231:ARG:NH1	3:D:142:GLU:CD	2.60	0.54
7:E:1237:AMP:H5'1	8:E:2117:HOH:O	2.08	0.54
2:E:226:MET:HE1	3:F:111:GLY:HA3	1.90	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
2:E:226:MET:HE3	3:F:148:LYS:NZ	2.23	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
2:C:226:MET:HE3	2:C:226:MET:HA	1.91	0.53
3:D:19:LEU:HA	3:D:22:ILE:HD12	1.89	0.53
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
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
2:C:226:MET:HE2	3:D:111:GLY:HA2	1.90	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:190:LYS:NZ	8:A:2216:HOH:O	2.44	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
2:C:54:ASP:CA	2:C:56:ASP:N	2.73	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:280:ILE:HD12	8:A:2334:HOH:O	2.13	0.48
1:B:295:LEU:C	1:B:295:LEU:HD12	2.34	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
2:E:102:ARG:O	2:E:102:ARG:HG3	2.13	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
1:B:139:MET:HE2	1:B:144:ILE:HA	1.96	0.47
1:B:60:TYR:CE2	1:B:74:SER:HA	2.49	0.47
2:C:1:MET:HE3	8:C:2130:HOH:O	2.07	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
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
1:B:139:MET:CE	1:B:144:ILE:HA	2.46	0.45
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
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
2:C:195:ARG:NH1	8:C:2156:HOH:O	2.49	0.45
3:D:76:GLU:CD	3:D:105:SER:HG	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:MET:HG2	2:C:57:VAL:HG22	2.00	0.44
2:E:1:MET:HE2	8:E:2116:HOH:O	2.15	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
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:C:226:MET:HE1	3:D:111:GLY:HA2	1.99	0.43
2:E:230:ARG:NH2	3:F:124:GLN:NE2	2.63	0.43
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
2:E:28:GLU:HA	2:E:31:MET:HE3	2.01	0.42
1:A:121:ARG:HH22	1:A:146:GLN:NE2	2.18	0.42
3:D:76:GLU:CD	3:D:105:SER:OG	2.58	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:118:ALA:O	2:C:181:THR:HA	2.18	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
2:E:24:MET:O	2:E:232:MET:HE3	2.21	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:77:ILE:HD12	1:A:77:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:76:GLU:OE2	3:D:109:LYS:NZ	2.52	0.40
2:C:1:MET:HE2	2:C:114:ASP:CG	2.41	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
2:C:25:ASP:HA	2:C:232:MET:CE	2.34	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
2:C:176:CYS:HA	2:C:177:PRO:C	2.41	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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%)	12	6
2	E	234/264 (89%)	230 (98%)	4 (2%)	0	100	100
3	D	187/320 (58%)	179 (96%)	7 (4%)	1 (0%)	29	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	187/320 (58%)	184 (98%)	3 (2%)	0	100	100
All	All	2291/2626 (87%)	2217 (97%)	70 (3%)	4 (0%)	47	44

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%)	574 (98%)	10 (2%)	60	65
1	B	578/602 (96%)	565 (98%)	13 (2%)	52	55
2	C	180/216 (83%)	171 (95%)	9 (5%)	24	20
2	E	177/216 (82%)	171 (97%)	6 (3%)	37	36
3	D	143/258 (55%)	134 (94%)	9 (6%)	18	13
3	F	150/258 (58%)	141 (94%)	9 (6%)	19	14
All	All	1812/2152 (84%)	1756 (97%)	56 (3%)	40	40

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	40	PHE
1	A	60	TYR
1	A	330	LEU
1	A	444	ARG
1	A	589	LEU
1	A	631	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	650	LEU
1	A	667	LYS
1	A	718	MET
1	B	26	GLN
1	B	40	PHE
1	B	60	TYR
1	B	71	HIS
1	B	203	LEU
1	B	253	MET
1	B	441	SER
1	B	444	ARG
1	B	589	LEU
1	B	601	ARG
1	B	615	THR
1	B	650	LEU
1	B	667	LYS
2	C	1	MET
2	C	32	MET
2	C	56	ASP
2	C	89	ASP
2	C	96	ASP
2	C	156	ASN
2	C	157	LYS
2	C	228	ARG
2	C	231	ARG
3	D	21	LEU
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	102	ARG
2	E	156	ASN
2	E	157	LYS
2	E	183	GLN
2	E	226	MET
3	F	29	LYS
3	F	37	VAL

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Mol	Chain	Res	Type
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	288	GLN
1	A	535	ASN
1	A	563	HIS
1	B	26	GLN
1	B	276	GLN
1	B	563	HIS
1	B	652	ASN
2	C	121	GLN
2	C	150	GLN
2	C	170	GLN
2	C	175	ASN
2	C	183	GLN
2	C	199	GLN
3	D	44	GLN
3	D	124	GLN
3	D	137	GLN
3	D	173	ASN
3	D	184	GLN
2	E	150	GLN
2	E	170	GLN
2	E	175	ASN
2	E	183	GLN
2	E	199	GLN
3	F	26	ASN
3	F	44	GLN
3	F	124	GLN
3	F	137	GLN
3	F	180	GLN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
6	SF4	B	1732	1	0,12,12	-	-	-	-	-
4	FMN	B	1730	1	33,33,33	1.45	6 (18%)	48,50,50	1.50	9 (18%)
5	ADP	B	1731	-	24,29,29	1.27	2 (8%)	29,45,45	1.42	3 (10%)
7	AMP	E	1237	-	22,25,25	1.87	5 (22%)	25,38,38	3.00	11 (44%)
6	SF4	A	1732	1	0,12,12	-	-	-	-	-
7	AMP	C	1236	-	22,25,25	1.44	3 (13%)	25,38,38	2.71	9 (36%)
4	FMN	A	1730	1	33,33,33	1.34	6 (18%)	48,50,50	1.56	10 (20%)
5	ADP	A	1731	-	24,29,29	1.25	1 (4%)	29,45,45	1.36	4 (13%)

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
6	SF4	B	1732	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	B	1730	1	-	1/18/18/18	0/3/3/3
5	ADP	B	1731	-	-	3/12/32/32	0/3/3/3
7	AMP	E	1237	-	-	4/6/26/26	0/3/3/3
6	SF4	A	1732	1	-	-	0/6/5/5
7	AMP	C	1236	-	-	4/6/26/26	0/3/3/3
4	FMN	A	1730	1	-	1/18/18/18	0/3/3/3
5	ADP	A	1731	-	-	3/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1237	AMP	C2-N3	5.89	1.41	1.32
7	C	1236	AMP	C2-N3	4.67	1.39	1.32
5	A	1731	ADP	C2-N3	4.47	1.39	1.32
5	B	1731	ADP	C2-N3	3.81	1.38	1.32
4	A	1730	FMN	C4A-N5	3.62	1.37	1.30
7	E	1237	AMP	C2'-C1'	-3.09	1.49	1.53
7	E	1237	AMP	C2-N1	2.96	1.39	1.33
4	B	1730	FMN	C9A-N10	-2.77	1.36	1.41
7	C	1236	AMP	C2-N1	2.67	1.38	1.33
4	B	1730	FMN	C1'-C2'	2.64	1.56	1.52
4	B	1730	FMN	C4A-N5	2.58	1.35	1.30
4	A	1730	FMN	C10-N1	2.55	1.38	1.33
7	E	1237	AMP	O4'-C4'	-2.41	1.39	1.45
7	E	1237	AMP	O5'-C5'	-2.39	1.35	1.44
7	C	1236	AMP	O5'-C5'	-2.39	1.35	1.44
4	B	1730	FMN	C9-C8	-2.29	1.36	1.39
4	A	1730	FMN	C9-C8	-2.24	1.36	1.39
4	B	1730	FMN	C5'-C4'	2.22	1.54	1.51
5	B	1731	ADP	C2-N1	2.10	1.37	1.33
4	A	1730	FMN	C6-C5A	-2.09	1.36	1.40
4	A	1730	FMN	C6-C7	2.01	1.42	1.39
4	B	1730	FMN	C6-C5A	-2.01	1.36	1.40
4	A	1730	FMN	C1'-N10	2.00	1.53	1.48

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	1237	AMP	P-O5'-C5'	8.80	142.53	118.30
7	C	1236	AMP	N3-C2-N1	-6.64	118.29	128.68
7	C	1236	AMP	O2P-P-O5'	6.40	123.76	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1236	AMP	P-O5'-C5'	6.38	135.86	118.30
7	E	1237	AMP	N3-C2-N1	-6.22	118.96	128.68
7	E	1237	AMP	O2P-P-O5'	5.10	120.29	106.73
5	A	1731	ADP	N3-C2-N1	-4.95	120.94	128.68
5	B	1731	ADP	N3-C2-N1	-4.94	120.95	128.68
7	E	1237	AMP	O5'-P-O1P	-4.28	94.48	106.47
7	C	1236	AMP	O5'-P-O1P	-3.97	95.33	106.47
4	A	1730	FMN	C9A-C5A-N5	-3.49	118.64	122.43
7	E	1237	AMP	C4-C5-N7	-3.47	105.78	109.40
7	E	1237	AMP	C5-C6-N6	3.37	125.47	120.35
4	B	1730	FMN	C10-C4A-N5	-3.25	117.95	124.86
4	A	1730	FMN	C6-C5A-N5	3.15	124.01	118.51
4	B	1730	FMN	C4A-C10-N10	3.04	120.93	116.48
4	A	1730	FMN	O4-C4-C4A	-3.02	118.60	126.60
4	B	1730	FMN	C6-C5A-N5	2.91	123.59	118.51
4	A	1730	FMN	C8M-C8-C9	-2.88	114.17	119.49
4	B	1730	FMN	C9A-C5A-N5	-2.76	119.43	122.43
5	A	1731	ADP	C4-C5-N7	-2.75	106.53	109.40
5	B	1731	ADP	O3B-PB-O3A	2.73	113.78	104.64
4	B	1730	FMN	O4-C4-C4A	-2.72	119.39	126.60
7	E	1237	AMP	C2'-C3'-C4'	-2.60	97.59	102.64
4	A	1730	FMN	C4A-C10-N10	2.58	120.25	116.48
4	A	1730	FMN	C5A-C9A-N10	2.53	120.57	117.95
7	C	1236	AMP	C2-N1-C6	2.52	123.07	118.75
4	B	1730	FMN	C7M-C7-C8	-2.51	115.59	120.74
7	E	1237	AMP	C3'-C2'-C1'	2.50	104.74	100.98
7	E	1237	AMP	C5'-C4'-C3'	2.47	124.44	115.18
7	E	1237	AMP	O2'-C2'-C1'	-2.47	101.74	110.85
7	E	1237	AMP	C2-N1-C6	2.44	122.92	118.75
7	C	1236	AMP	C5-C6-N6	2.38	123.97	120.35
4	B	1730	FMN	C4-C4A-C10	2.38	120.78	116.79
4	A	1730	FMN	C7M-C7-C8	-2.33	115.96	120.74
4	A	1730	FMN	C9A-C9-C8	2.32	123.97	119.30
7	C	1236	AMP	C4-C5-N7	-2.26	107.04	109.40
4	A	1730	FMN	C10-C4A-N5	-2.25	120.09	124.86
4	A	1730	FMN	C1'-C2'-C3'	2.24	116.05	109.79
5	A	1731	ADP	PA-O3A-PB	-2.20	125.28	132.83
7	C	1236	AMP	C5'-C4'-C3'	2.15	123.26	115.18
7	C	1236	AMP	O2'-C2'-C1'	-2.15	102.91	110.85
4	B	1730	FMN	C4-C4A-N5	2.13	121.26	118.23
4	B	1730	FMN	C5A-N5-C4A	2.03	121.45	118.07
5	B	1731	ADP	C5-C6-N6	2.01	123.41	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1731	ADP	C1'-N9-C4	-2.01	123.11	126.64

There are no chirality outliers.

All (16) 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	E	1237	AMP	C3'-C4'-C5'-O5'
7	C	1236	AMP	C5'-O5'-P-O1P
7	E	1237	AMP	C5'-O5'-P-O1P
4	A	1730	FMN	C4'-C5'-O5'-P
4	B	1730	FMN	C4'-C5'-O5'-P
7	E	1237	AMP	C5'-O5'-P-O2P
5	B	1731	ADP	PB-O3A-PA-O2A
5	A	1731	ADP	PB-O3A-PA-O2A
5	A	1731	ADP	PB-O3A-PA-O1A
7	C	1236	AMP	C3'-C4'-C5'-O5'
5	B	1731	ADP	PB-O3A-PA-O1A
5	A	1731	ADP	O4'-C4'-C5'-O5'
5	B	1731	ADP	O4'-C4'-C5'-O5'

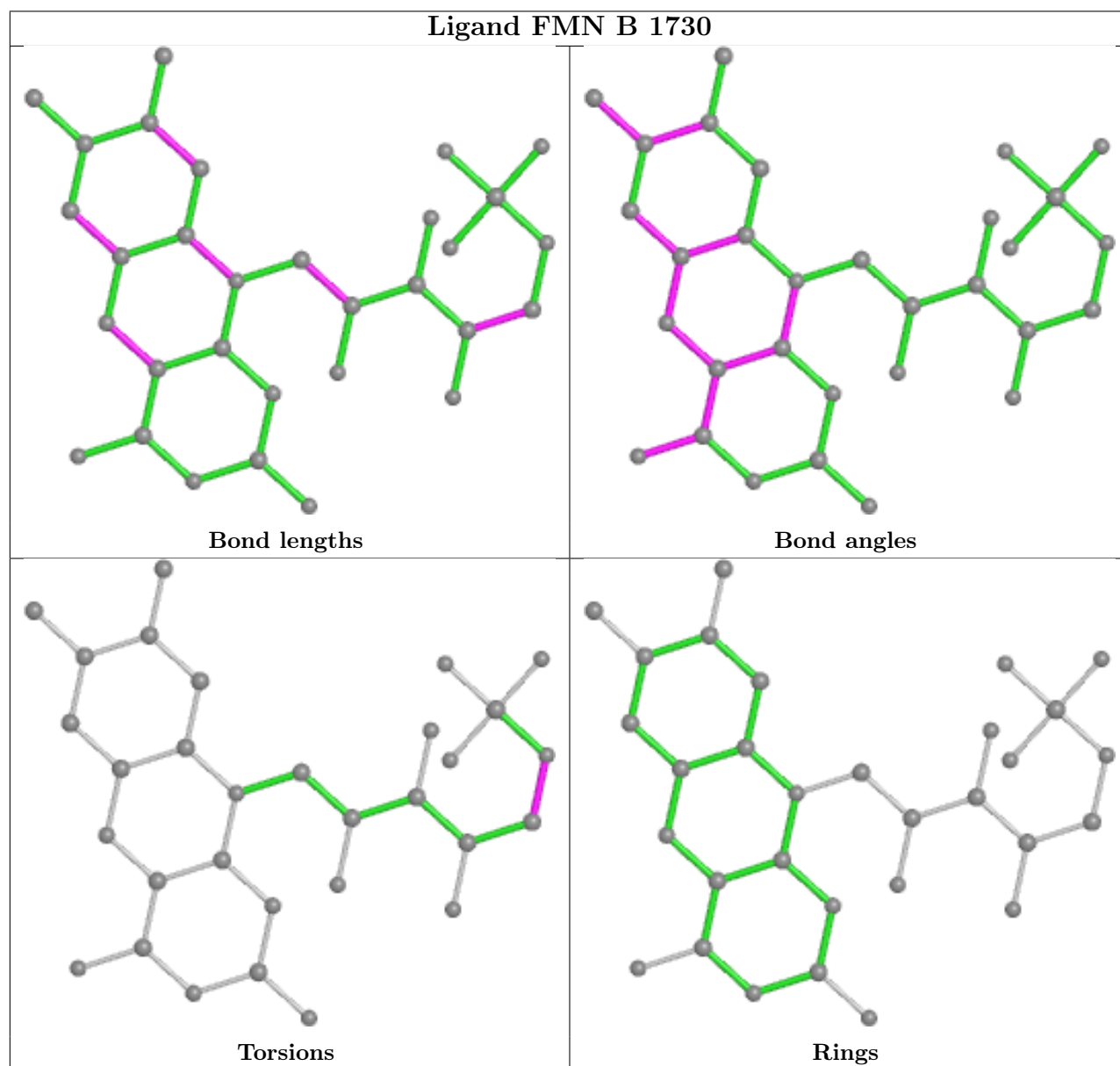
There are no ring outliers.

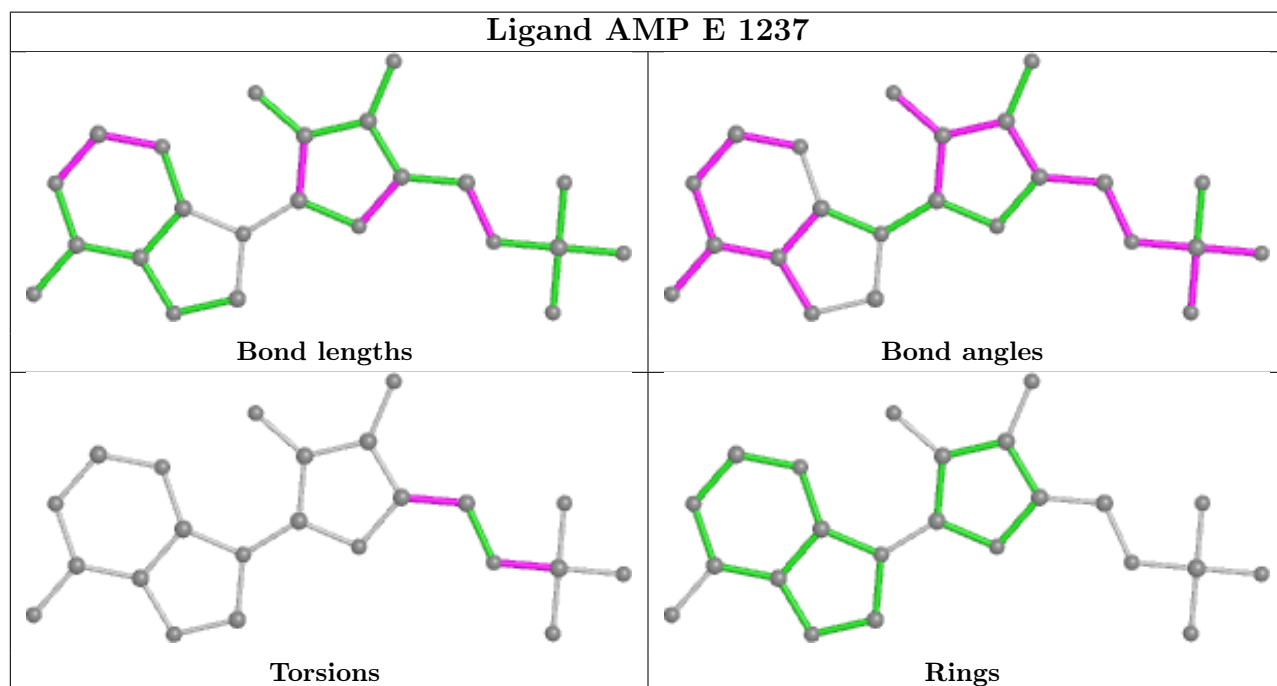
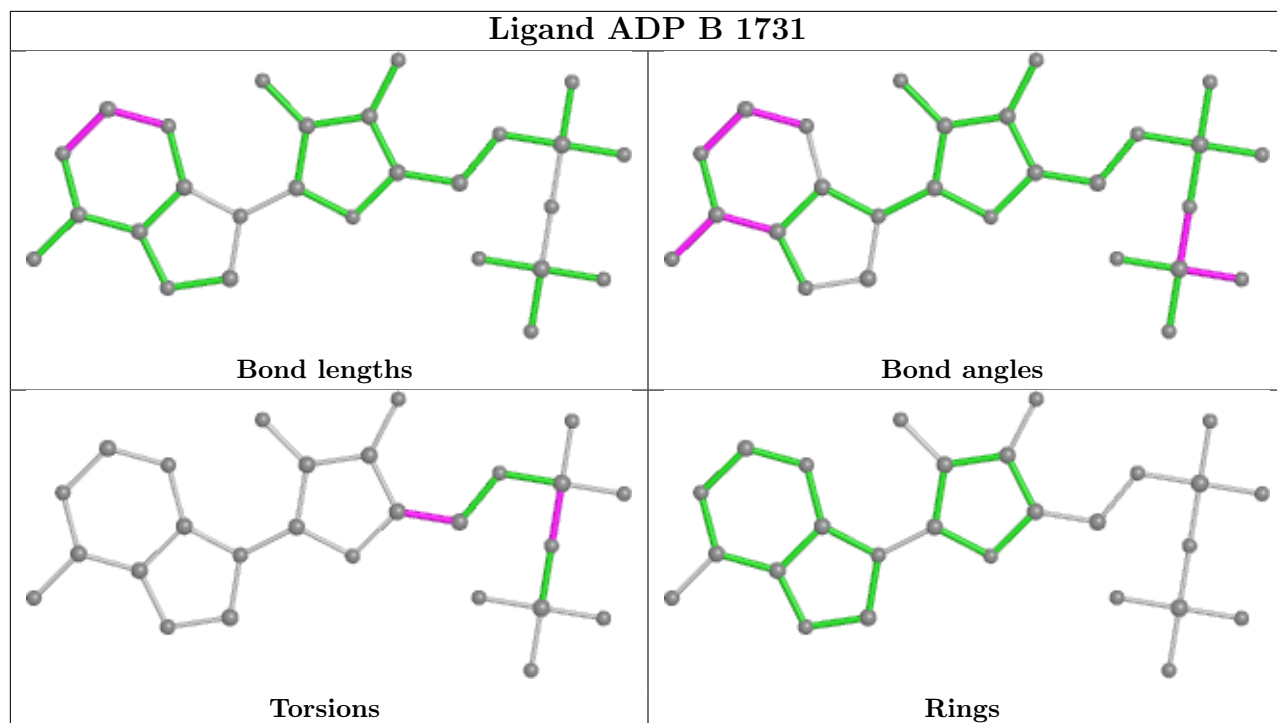
4 monomers are involved in 6 short contacts:

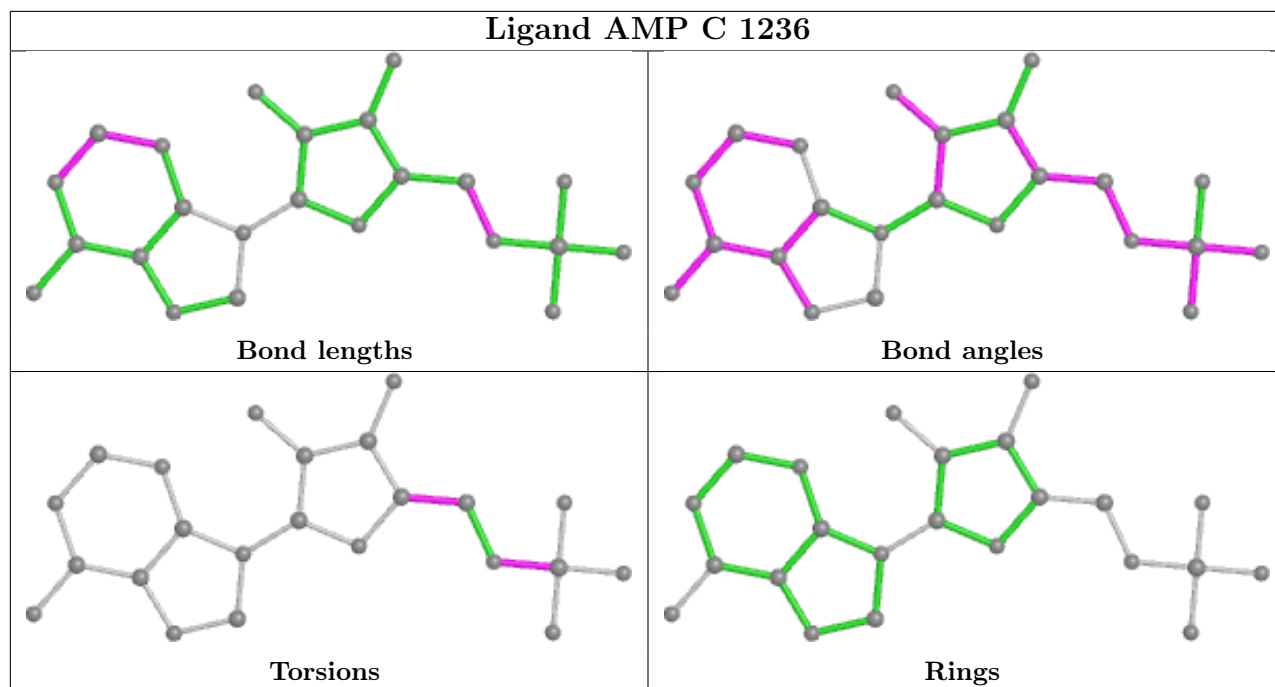
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1732	SF4	2	0
4	B	1730	FMN	1	0
7	E	1237	AMP	1	0
7	C	1236	AMP	2	0

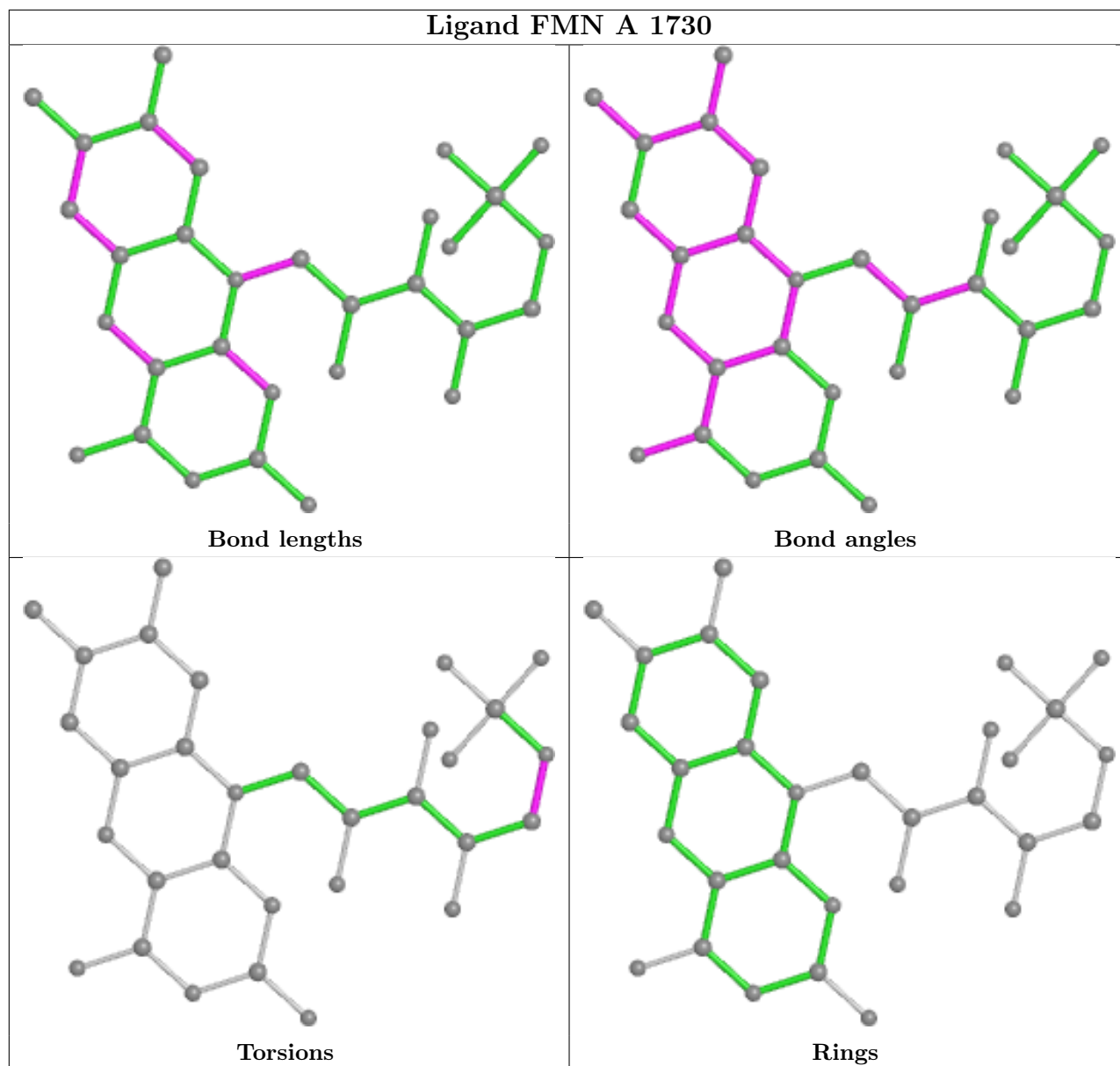
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

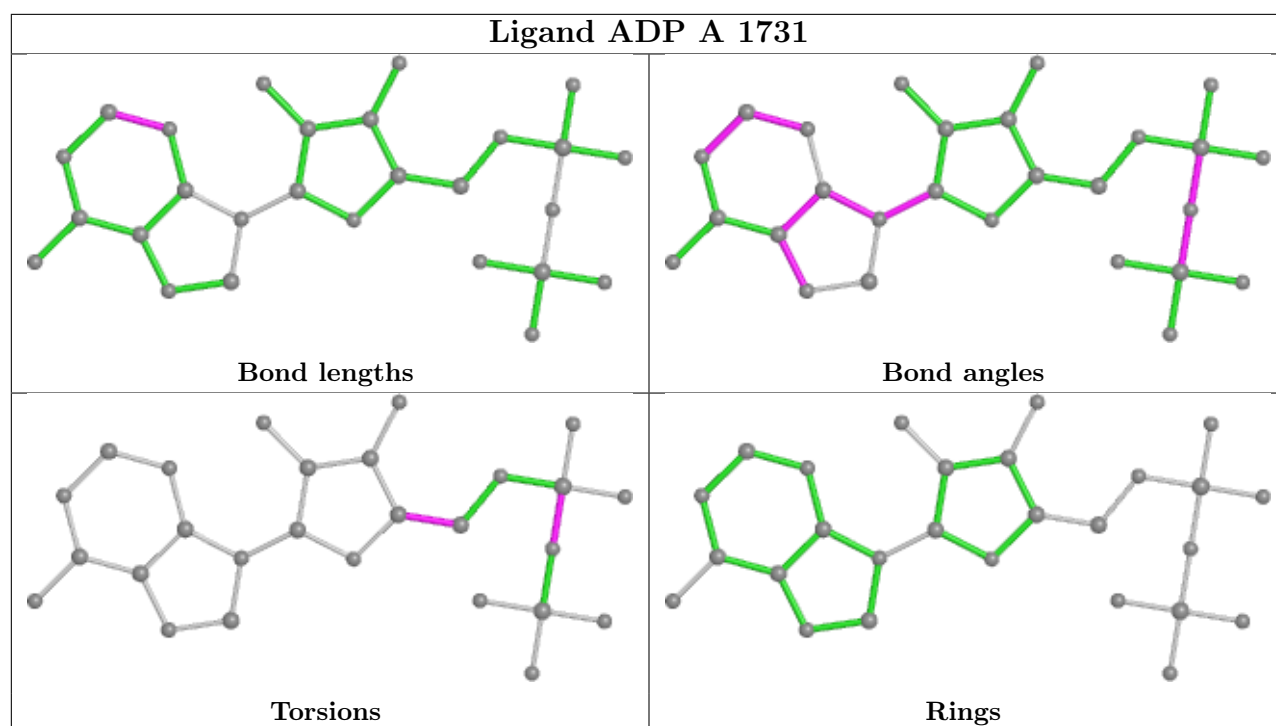












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	729/729 (100%)	-0.50	0 <b>100</b> <b>100</b>	21, 28, 40, 47	0
1	B	729/729 (100%)	-0.58	3 (0%) <b>92</b> <b>92</b>	18, 26, 38, 53	0
2	C	233/264 (88%)	-0.21	3 (1%) <b>77</b> <b>76</b>	25, 35, 56, 66	0
2	E	236/264 (89%)	-0.19	6 (2%) <b>57</b> <b>56</b>	25, 33, 50, 58	0
3	D	189/320 (59%)	0.52	22 (11%) <b>4</b> <b>4</b>	32, 50, 66, 76	0
3	F	189/320 (59%)	-0.14	6 (3%) <b>47</b> <b>46</b>	27, 36, 52, 63	0
All	All	2305/2626 (87%)	-0.35	40 (1%) <b>70</b> <b>68</b>	18, 30, 53, 76	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	177	PRO	6.2
3	D	125	GLY	5.2
3	D	31	SER	4.9
3	F	32	GLY	4.6
3	D	32	GLY	4.3
3	D	126	ASP	4.2
3	F	31	SER	4.2
3	D	176	ALA	4.0
2	E	54	ASP	3.9
3	D	174	VAL	3.6
3	D	147	GLY	3.5
3	D	34	ASP	3.3
3	D	178	SER	3.2
3	D	168	SER	3.1
1	B	1	ALA	3.1
3	D	175	ASP	3.1
2	E	217	ALA	3.0
2	E	236	GLU	3.0
3	D	84	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	66	SER	3.0
3	D	33	GLU	2.9
2	E	166	GLY	2.9
3	D	30	LYS	2.8
2	C	53	SER	2.7
3	D	170	VAL	2.6
3	D	149	SER	2.5
1	B	601	ARG	2.5
2	E	16	ASP	2.3
3	D	180	GLN	2.3
3	D	179	VAL	2.3
3	F	178	SER	2.2
3	F	147	GLY	2.2
2	C	29	ASP	2.2
3	D	163	LEU	2.1
3	D	65	GLY	2.0
2	E	24	MET	2.0
1	B	563	HIS	2.0
3	F	125	GLY	2.0
3	F	126	ASP	2.0
2	C	56	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

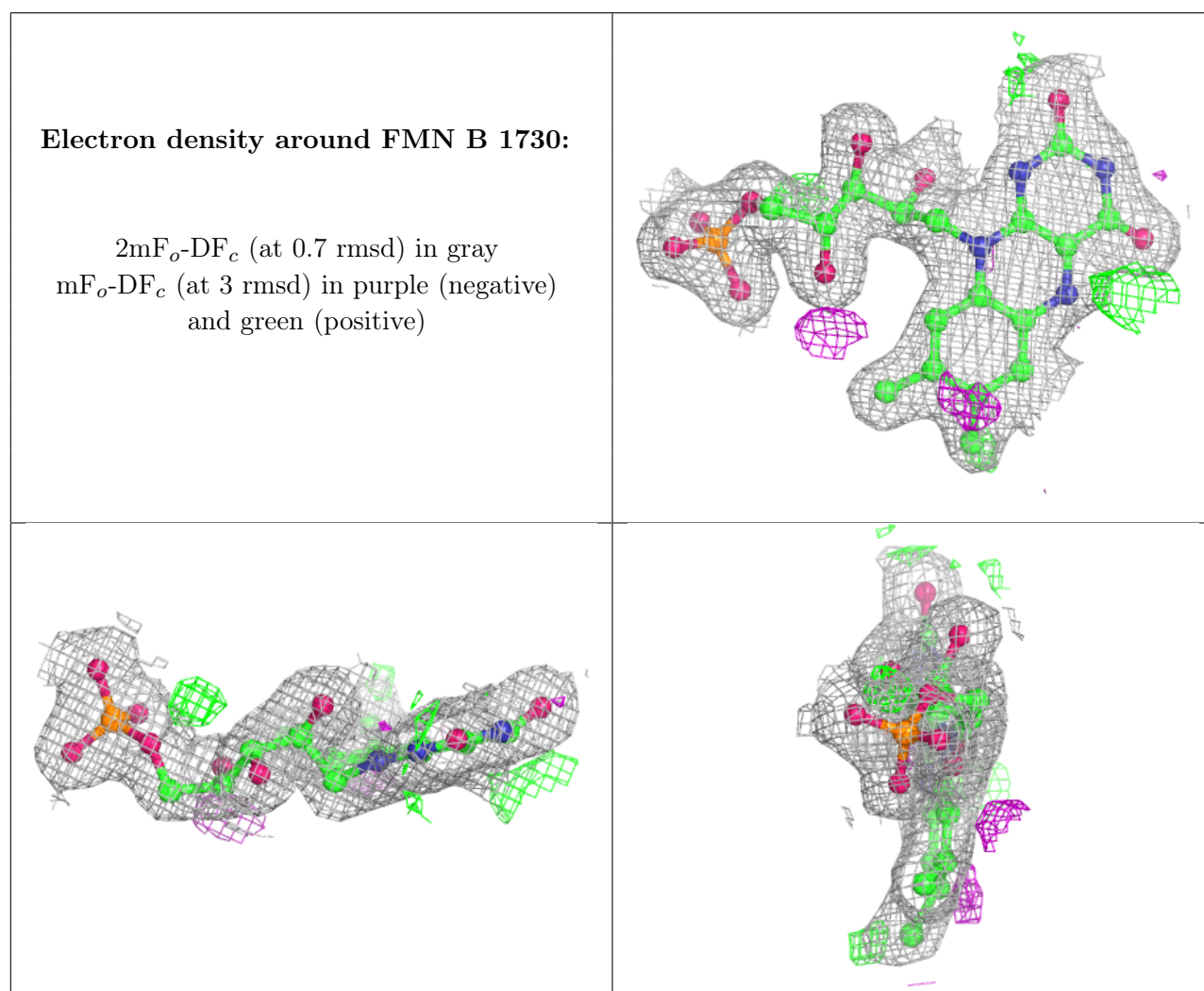
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q < 0.9
6	SF4	B	1732	8/8	0.87	0.14	28,29,43,49	0
4	FMN	B	1730	31/31	0.95	0.11	19,23,26,28	0

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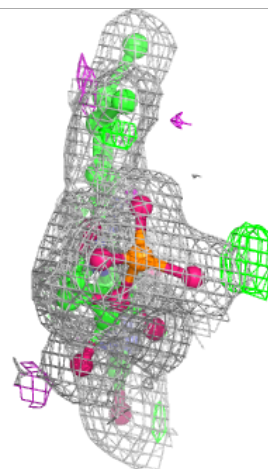
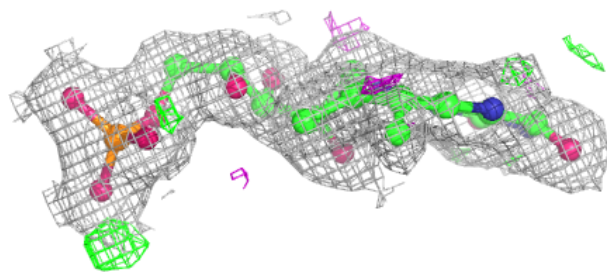
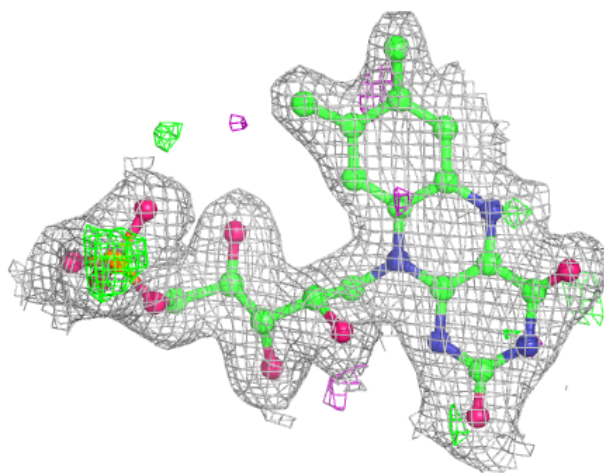
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SF4	A	1732	8/8	0.96	0.07	29,31,32,36	0
4	FMN	A	1730	31/31	0.96	0.09	18,23,25,27	0
7	AMP	C	1236	23/23	0.97	0.08	26,30,37,38	0
7	AMP	E	1237	23/23	0.97	0.09	23,28,33,35	0
5	ADP	A	1731	27/27	0.98	0.07	23,28,30,31	0
5	ADP	B	1731	27/27	0.99	0.06	20,24,28,29	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.



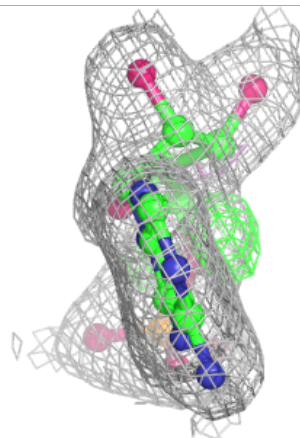
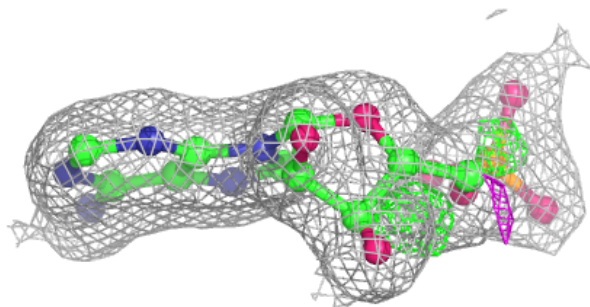
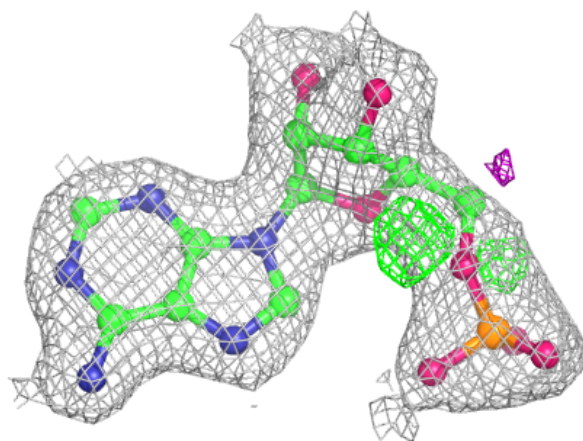
**Electron density around FMN A 1730:**

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



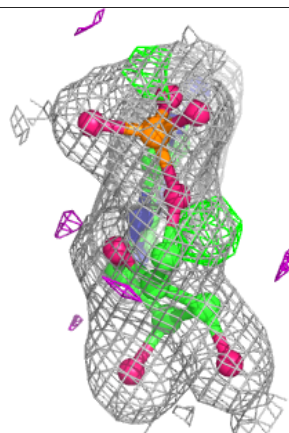
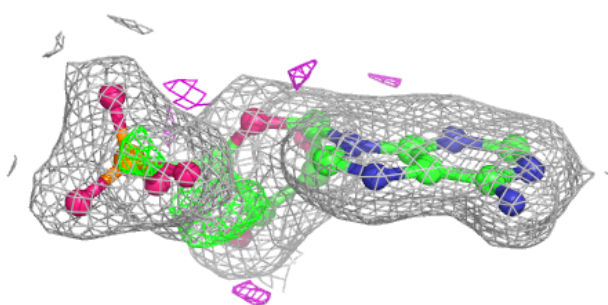
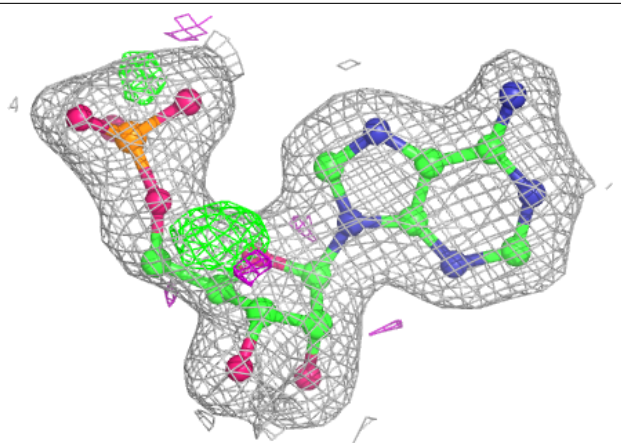
**Electron density around AMP C 1236:**

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

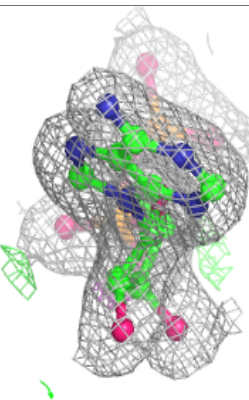
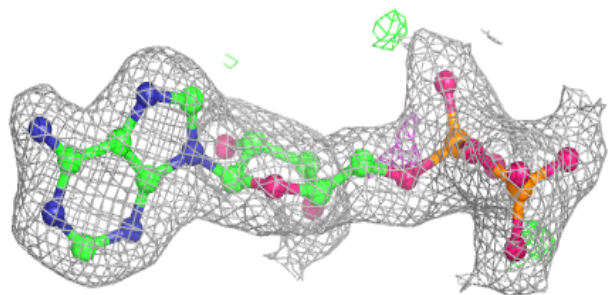
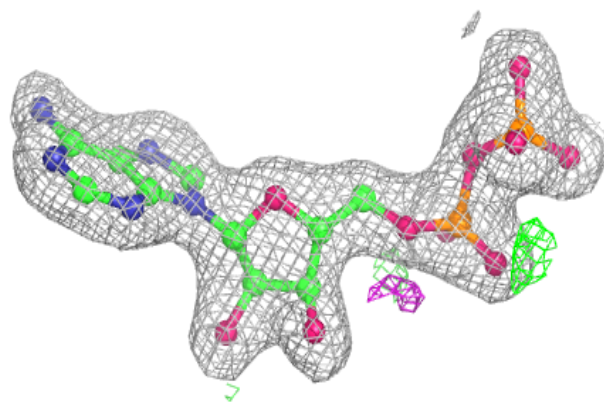


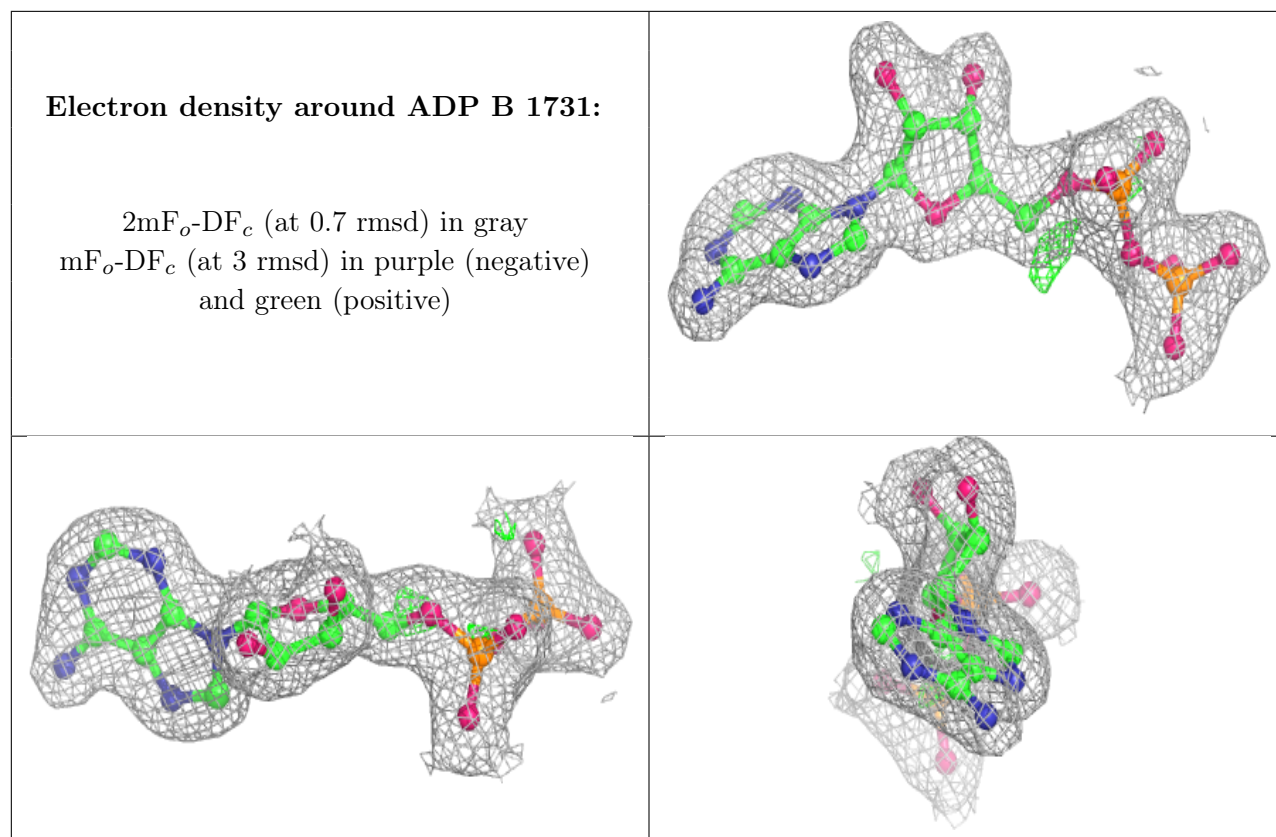
**Electron density around AMP E 1237:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.