



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 02:22 PM EDT

PDB ID : 3FGC  
Title : Crystal Structure of the Bacterial Luciferase:Flavin Complex Reveals the Basis of Intersubunit Communication  
Authors : Campbell, Z.T.; Weichsel, A.; Montfort, W.R.; Baldwin, T.O.  
Deposited on : 2008-12-05  
Resolution : 2.30 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

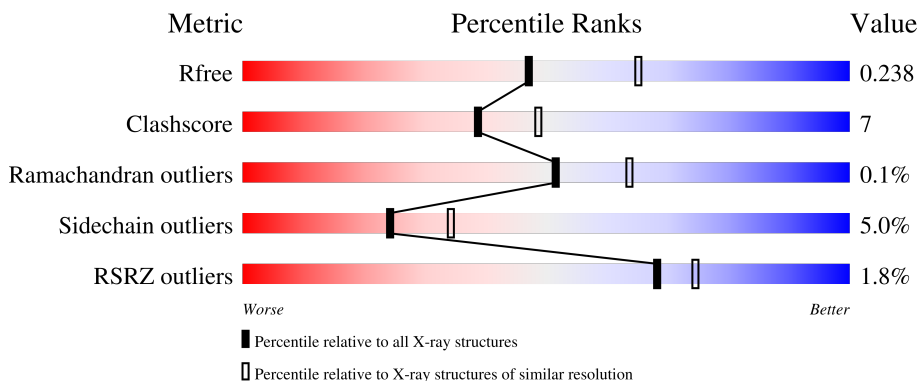
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	355	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">2%      78%      19%      ..</p>
1	C	355	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">3%      81%      15%      ..</p>
2	B	332	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">%      85%      9%      . .</p>
2	D	332	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">%      81%      15%      ..</p>

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
4	PO4	A	356[B]	-	X	-	-
4	PO4	C	359	-	-	X	-
5	SO4	A	361	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11895 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 Alkanal monooxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2832	1797	471	546	18	0	7	0
1	C	348	2849	1809	470	552	18	0	11	0

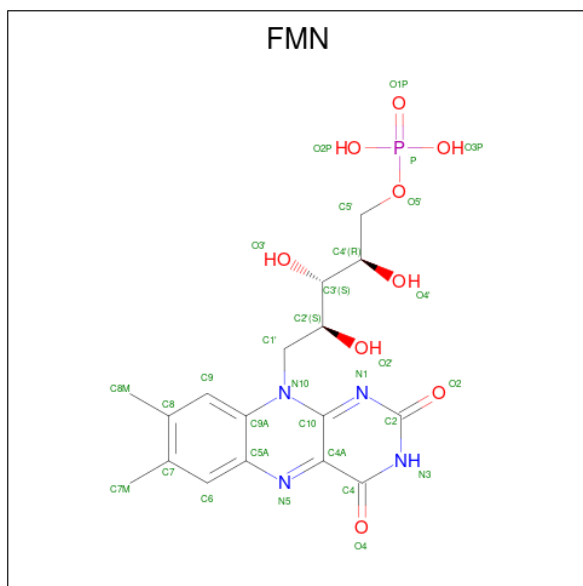
- Molecule 2 is a protein called Alkanal monooxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	318	2550	1601	440	494	15	0	5	0
2	D	325	2696	1695	465	521	15	0	15	0

There are 16 discrepancies between the modelled and reference sequences:

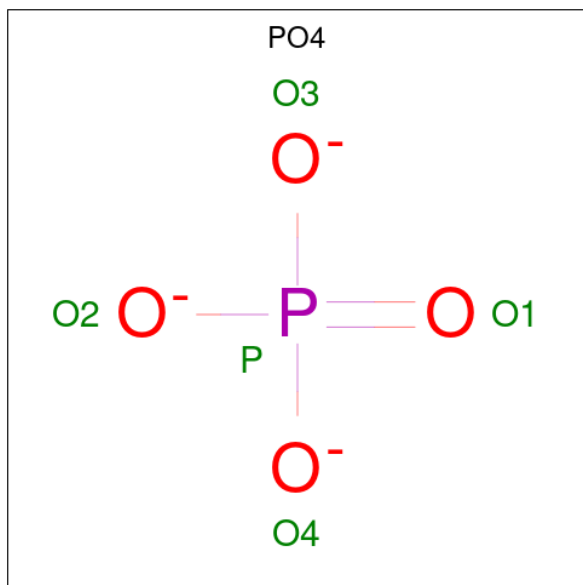
Chain	Residue	Modelled	Actual	Comment	Reference
B	325	LEU	-	expression tag	UNP P07739
B	326	GLU	-	expression tag	UNP P07739
B	327	HIS	-	expression tag	UNP P07739
B	328	HIS	-	expression tag	UNP P07739
B	329	HIS	-	expression tag	UNP P07739
B	330	HIS	-	expression tag	UNP P07739
B	331	HIS	-	expression tag	UNP P07739
B	332	HIS	-	expression tag	UNP P07739
D	325	LEU	-	expression tag	UNP P07739
D	326	GLU	-	expression tag	UNP P07739
D	327	HIS	-	expression tag	UNP P07739
D	328	HIS	-	expression tag	UNP P07739
D	329	HIS	-	expression tag	UNP P07739
D	330	HIS	-	expression tag	UNP P07739
D	331	HIS	-	expression tag	UNP P07739
D	332	HIS	-	expression tag	UNP P07739

- Molecule 3 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
			Total	C	N	O	P		
3	A	1	31	17	4	9	1	0	1

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	5	4	1	0	1
4	C	1	5	4	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

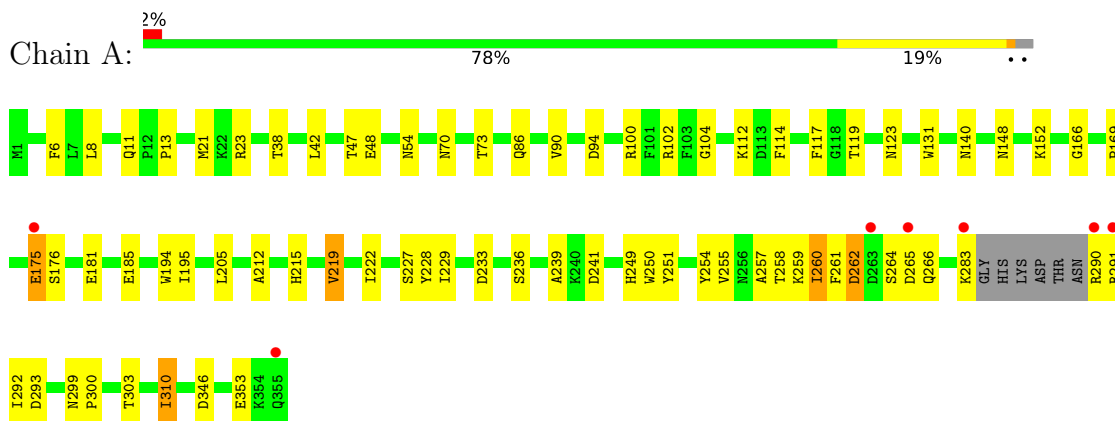
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	251	Total	O	0	21
			272	272		
6	B	218	Total	O	1	14
			233	233		
6	C	133	Total	O	0	10
			144	144		
6	D	179	Total	O	0	19
			198	198		

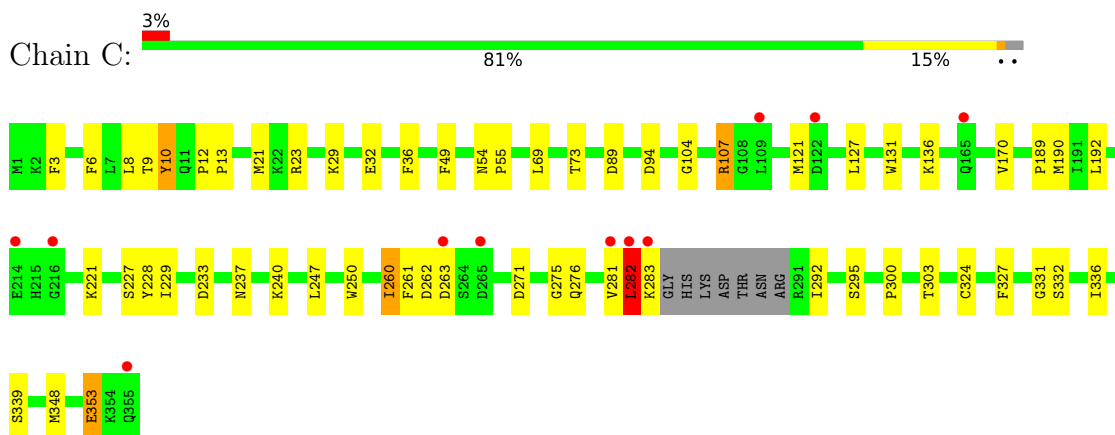
### 3 Residue-property plots

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.

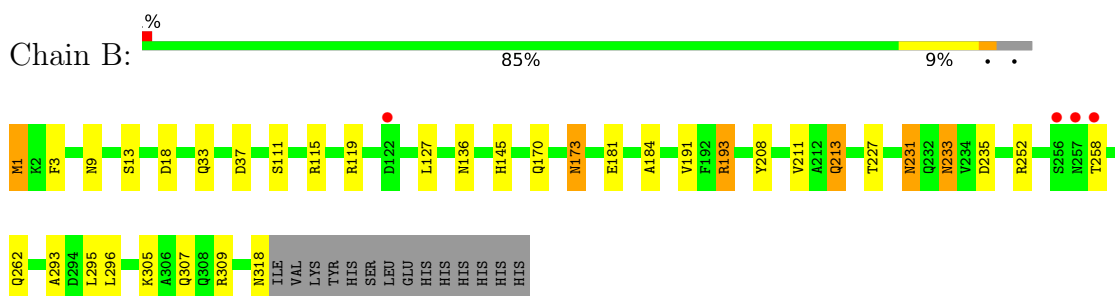
- Molecule 1: Alkanal monooxygenase alpha chain



- Molecule 1: Alkanal monooxygenase alpha chain




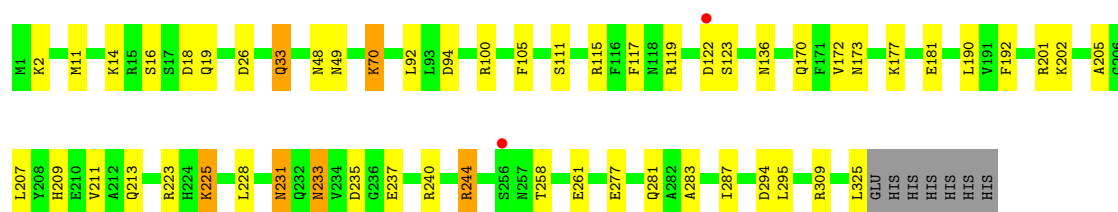
- Molecule 2: Alkanal monooxygenase beta chain





- Molecule 2: Alkanal monooxygenase beta chain

Chain D:  %



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.89Å 109.30Å 301.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.33 – 2.30 27.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.33-2.30) 99.9 (27.33-2.30)	Depositor EDS
$R_{merge}$	0.43	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.35 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.184 , 0.241 0.185 , 0.238	Depositor DCC
$R_{free}$ test set	4385 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtrriage
Anisotropy	0.070	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PO4, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.01	3/2905 (0.1%)	0.88	3/3935 (0.1%)
1	C	0.85	0/2933	0.79	2/3974 (0.1%)
2	B	0.98	0/2607	0.81	0/3525
2	D	0.92	0/2753	0.77	1/3720 (0.0%)
All	All	0.94	3/11198 (0.0%)	0.81	6/15154 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	PHE	CE2-CZ	5.65	1.48	1.37
1	A	219	VAL	CB-CG2	5.28	1.64	1.52
1	A	212	ALA	CA-CB	5.14	1.63	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASP	CB-CG-OD1	5.97	123.68	118.30
2	D	94	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	21	MET	CG-SD-CE	-5.67	91.13	100.20
1	A	241	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	282	LEU	CA-CB-CG	5.31	127.51	115.30
1	C	94	ASP	CB-CG-OD2	-5.17	113.65	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2832	0	2710	45	0
1	C	2849	0	2709	54	0
2	B	2550	0	2426	28	0
2	D	2696	0	2566	39	0
3	A	31	0	19	1	0
4	A	5	0	0	1	0
4	C	5	0	0	2	0
5	A	25	0	0	2	0
5	B	15	0	0	1	0
5	C	15	0	0	0	0
5	D	25	0	0	0	0
6	A	272	0	0	2	0
6	B	233	0	0	7	0
6	C	144	0	0	5	0
6	D	198	0	0	4	0
All	All	11895	0	10430	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10[B]:TYR:CD2	1:C:250[B]:TRP:HZ3	1.65	1.15
1:C:10[B]:TYR:CD2	1:C:250[B]:TRP:CZ3	2.37	1.11
2:D:16:SER:OG	2:D:19[A]:GLN:HG3	1.57	1.04
2:D:181:GLU:HG3	2:D:211:VAL:HG21	1.41	0.98
2:B:173:ASN:ND2	2:B:193:ARG:HD2	1.81	0.96
2:B:181:GLU:HG3	2:B:211:VAL:HG21	1.47	0.95
1:A:6[A]:PHE:CE2	1:A:227:SER:HB2	2.02	0.94
1:A:112:LYS:HB3	1:A:260:ILE:HD11	1.48	0.93
1:A:6[A]:PHE:HE2	1:A:227:SER:HB2	1.38	0.88
1:C:10[B]:TYR:HD2	1:C:250[B]:TRP:HZ3	1.22	0.85
1:A:175[B]:GLU:CA	1:A:176:SER:N	2.42	0.82
1:C:282:LEU:HD13	1:C:283:LYS:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:205:ALA:O	2:D:209[B]:HIS:CD2	2.36	0.78
1:C:262:ASP:O	1:C:263:ASP:HB2	1.84	0.76
1:A:249:HIS:HE1	6:D:354:HOH:O	1.70	0.74
1:C:237:ASN:ND2	6:C:400:HOH:O	2.21	0.74
2:D:205:ALA:O	2:D:209[B]:HIS:HD2	1.71	0.74
2:B:173:ASN:HD21	2:B:193:ARG:HD2	1.54	0.72
1:C:107:ARG:HG3	6:C:380:HOH:O	1.90	0.72
1:A:175[B]:GLU:CA	1:A:175[B]:GLU:O	2.40	0.70
1:A:175[B]:GLU:O	1:A:176:SER:N	2.25	0.70
1:C:136[A]:LYS:HE2	6:C:422:HOH:O	1.92	0.68
1:C:32:GLU:HB2	1:C:69:LEU:HD13	1.77	0.67
1:A:299:ASN:O	1:A:310:ILE:HD13	1.96	0.66
2:B:233:ASN:HD22	2:B:235:ASP:H	1.44	0.65
1:C:49:PHE:O	1:C:250[B]:TRP:CH2	2.49	0.65
1:A:175[B]:GLU:O	1:A:175[B]:GLU:CD	2.37	0.62
2:D:16:SER:H	2:D:19[A]:GLN:HE21	1.47	0.62
1:C:23:ARG:NH2	1:C:331:GLY:O	2.33	0.62
1:C:10[B]:TYR:CD2	1:C:250[B]:TRP:CE3	2.88	0.61
1:C:282:LEU:CD1	1:C:283:LYS:H	2.13	0.61
1:C:6[B]:PHE:CE2	1:C:227[B]:SER:HB2	2.36	0.60
2:B:252:ARG:HD2	6:B:353:HOH:O	2.01	0.60
1:C:271:ASP:O	1:C:275:GLY:CA	2.50	0.60
2:B:173:ASN:ND2	2:B:193:ARG:CD	2.61	0.60
2:D:181:GLU:HG3	2:D:211:VAL:CG2	2.24	0.60
2:D:277:GLU:HG2	2:D:281:GLN:NE2	2.18	0.59
1:C:8:LEU:HD13	1:C:250[B]:TRP:CZ2	2.37	0.59
2:D:244:ARG:NH2	2:D:261:GLU:OE2	2.36	0.58
1:C:21:MET:HE1	2:D:92:LEU:CD1	2.35	0.57
1:C:107:ARG:NH1	4:C:359:PO4:O2	2.38	0.57
1:C:55:PRO:HB2	1:C:73:THR:HG22	1.87	0.57
1:C:292:ILE:O	1:C:295[B]:SER:HB2	2.05	0.57
1:C:73:THR:O	1:C:104:GLY:HA3	2.04	0.56
2:B:233:ASN:ND2	2:B:235:ASP:H	2.03	0.56
1:C:233:ASP:O	1:C:303:THR:HA	2.06	0.56
1:C:271:ASP:O	1:C:275:GLY:HA2	2.05	0.56
2:B:111:SER:O	2:B:115[B]:ARG:HG3	2.05	0.56
2:D:172[A]:VAL:HG13	2:D:190:LEU:HD23	1.86	0.56
1:A:264:SER:HB2	5:A:361:SO4:O3	2.05	0.56
2:B:227:THR:HG22	2:B:296:LEU:HB2	1.87	0.56
1:C:3:PHE:CZ	1:C:348:MET:HG2	2.41	0.56
1:C:49:PHE:O	1:C:250[B]:TRP:CZ3	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LYS:NZ	6:C:400:HOH:O	2.39	0.55
1:C:260:ILE:HG23	1:C:261:PHE:CD1	2.42	0.55
2:D:2:LYS:HG3	2:D:223:ARG:NH2	2.21	0.55
1:C:332:SER:O	1:C:336:ILE:HG13	2.06	0.55
2:B:213:GLN:NE2	6:B:417:HOH:O	2.39	0.55
2:D:26[A]:ASP:OD2	2:D:309:ARG:NH2	2.35	0.54
2:D:233:ASN:HD22	2:D:235:ASP:H	1.54	0.54
2:D:136:ASN:HD22	2:D:170:GLN:HE22	1.54	0.54
1:A:254:TYR:O	1:A:258:THR:HG23	2.08	0.54
1:A:148:ASN:O	1:A:152:LYS:HE2	2.08	0.53
1:C:10[B]:TYR:CG	1:C:250[B]:TRP:CZ3	2.94	0.53
1:C:262:ASP:O	1:C:263:ASP:CB	2.56	0.53
2:B:231:ASN:C	2:B:231:ASN:HD22	2.11	0.53
1:A:6[A]:PHE:CZ	1:A:227:SER:HB2	2.42	0.52
1:C:228:TYR:CD1	1:C:300:PRO:HD3	2.45	0.52
1:C:121:MET:O	1:C:121:MET:HG2	2.09	0.52
2:B:307:GLN:HG3	6:B:713:HOH:O	2.11	0.51
2:B:136:ASN:HD22	2:B:170:GLN:HE22	1.58	0.51
2:B:193:ARG:HG2	2:B:193:ARG:HH11	1.75	0.51
1:C:21:MET:HE2	2:D:92:LEU:HD12	1.92	0.51
1:C:327:PHE:HD2	1:C:339[B]:SER:HG	1.59	0.51
1:C:21:MET:CE	2:D:92:LEU:HD12	2.40	0.51
2:D:117:PHE:O	2:D:119:ARG:NH1	2.42	0.51
1:A:102:ARG:HD3	1:A:169:PRO:HG2	1.94	0.50
2:D:237[A]:GLU:OE2	2:D:240:ARG:NE	2.41	0.50
2:B:173:ASN:HD21	2:B:193:ARG:CD	2.23	0.50
1:C:49:PHE:O	1:C:250[B]:TRP:HH2	1.92	0.50
1:A:175[B]:GLU:O	1:A:175[B]:GLU:OE1	2.30	0.49
2:D:237[A]:GLU:HG3	6:D:414:HOH:O	2.12	0.49
1:C:12:PRO:HB2	1:C:13:PRO:HD2	1.94	0.49
1:C:221:LYS:NZ	6:C:738:HOH:O	2.46	0.49
2:B:33:GLN:HB2	6:B:705:HOH:O	2.13	0.49
2:B:173:ASN:HD22	2:B:191:VAL:HG13	1.78	0.49
2:D:177:LYS:HG2	2:D:207:LEU:HD22	1.95	0.49
1:A:260:ILE:HD13	1:A:261:PHE:H	1.78	0.48
2:D:287:ILE:HD11	2:D:295:LEU:HD22	1.96	0.48
1:C:107:ARG:HD2	4:C:359:PO4:O3	2.15	0.47
1:C:327:PHE:HD2	1:C:339[B]:SER:OG	1.98	0.47
2:D:237[A]:GLU:CD	2:D:240:ARG:HE	2.18	0.47
2:D:111:SER:OG	2:D:115[B]:ARG:NH2	2.47	0.47
1:A:257:ALA:O	1:A:260:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:MET:CE	2:D:92:LEU:CD1	2.93	0.46
2:B:3:PHE:HA	2:B:295:LEU:O	2.16	0.46
1:A:175[B]:GLU:N	1:A:176:SER:N	2.61	0.46
2:B:193:ARG:NH2	6:B:426:HOH:O	2.45	0.46
1:A:86:GLN:O	1:A:90:VAL:HG23	2.16	0.46
1:A:260:ILE:HD12	1:A:260:ILE:H	1.81	0.46
2:D:225:LYS:HG3	2:D:294:ASP:HB2	1.97	0.45
1:A:23:ARG:NH1	6:A:383:HOH:O	2.49	0.45
2:B:145:HIS:ND1	5:B:335:SO4:O2	2.50	0.45
2:D:105:PHE:CZ	2:D:172[B]:VAL:HG22	2.52	0.45
2:D:231:ASN:C	2:D:231:ASN:HD22	2.20	0.45
1:A:8:LEU:HD13	1:A:250:TRP:CZ2	2.52	0.45
1:A:176:SER:N	4:A:356[B]:PO4:O3	2.50	0.44
1:A:194:TRP:CZ3	1:A:195:ILE:HG22	2.52	0.44
1:C:3:PHE:CE2	1:C:348:MET:HG2	2.52	0.44
1:A:215:HIS:HD2	6:A:586:HOH:O	2.00	0.44
2:D:33[A]:GLN:H	2:D:33[A]:GLN:HG2	1.53	0.44
1:A:114:PHE:CD2	1:A:119:THR:HG23	2.53	0.44
1:C:247:LEU:HD22	1:C:292:ILE:HD12	2.00	0.44
1:C:250[B]:TRP:CE3	1:C:250[B]:TRP:HA	2.52	0.44
1:C:32:GLU:HA	1:C:36:PHE:O	2.18	0.43
2:D:11:MET:O	2:D:48:ASN:HB3	2.18	0.43
1:A:73:THR:O	1:A:104:GLY:HA3	2.18	0.43
2:B:115[B]:ARG:NH1	6:B:376:HOH:O	2.51	0.43
2:B:1:MET:HA	2:B:293:ALA:O	2.19	0.43
1:C:190:MET:HE3	1:C:192:LEU:HD21	2.00	0.43
1:A:229[A]:ILE:HG22	1:A:299:ASN:CG	2.39	0.43
1:A:265:ASP:HB3	5:A:361:SO4:O4	2.19	0.43
2:D:192:PHE:HB3	2:D:201:ARG:HD2	2.01	0.43
2:B:181:GLU:HG2	2:B:211:VAL:HG11	2.00	0.43
1:A:236:SER:HB2	1:A:303:THR:HG23	2.00	0.43
1:C:250[A]:TRP:CZ3	1:C:292:ILE:HD13	2.54	0.43
1:A:181:GLU:O	1:A:185:GLU:HG3	2.19	0.42
1:C:6[B]:PHE:CE2	1:C:324:CYS:HB3	2.54	0.42
1:A:140:ASN:ND2	1:A:166:GLY:HA2	2.34	0.42
1:C:10[B]:TYR:CE2	1:C:250[B]:TRP:CE3	3.07	0.42
1:A:176:SER:N	3:A:3402[A]:FMN:O3P	2.52	0.42
1:A:251:TYR:O	1:A:255:VAL:HG23	2.19	0.42
2:D:49:ASN:ND2	6:D:701:HOH:O	2.51	0.42
2:B:184:ALA:HA	2:B:208:TYR:CE2	2.55	0.42
2:B:181:GLU:HG3	2:B:211:VAL:CG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HB3	1:A:48:GLU:HB2	2.02	0.42
2:D:244:ARG:HH22	2:D:261:GLU:CD	2.24	0.42
2:D:136:ASN:ND2	2:D:170:GLN:HE22	2.17	0.41
2:D:70[B]:LYS:HG2	2:D:100:ARG:O	2.20	0.41
1:C:353:GLU:H	1:C:353:GLU:HG2	1.62	0.41
2:B:9:ASN:ND2	6:B:549[A]:HOH:O	2.53	0.41
2:D:228:LEU:HD11	2:D:283:ALA:HA	2.02	0.41
1:A:233:ASP:O	1:A:303:THR:HA	2.20	0.41
2:B:305:LYS:O	2:B:309:ARG:HG2	2.21	0.41
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.92	0.41
2:D:223:ARG:NH2	2:D:294:ASP:OD1	2.46	0.41
1:A:13:PRO:O	2:D:202[A]:LYS:HD2	2.20	0.41
1:A:114:PHE:HD2	1:A:119:THR:HG23	1.86	0.41
1:A:228:TYR:CD1	1:A:300:PRO:HD3	2.56	0.41
1:A:259:LYS:O	1:A:262:ASP:HB2	2.21	0.41
1:C:170:VAL:O	1:C:189:PRO:HD2	2.21	0.41
1:A:38:THR:HA	1:A:70:ASN:O	2.21	0.40
1:C:10[B]:TYR:CE2	1:C:250[B]:TRP:CZ3	3.04	0.40
2:D:33[B]:GLN:HE21	2:D:33[B]:GLN:HB3	1.79	0.40
2:D:244:ARG:HD2	6:D:632:HOH:O	2.20	0.40
1:A:70:ASN:HD22	1:A:100:ARG:HB3	1.86	0.40
1:A:194:TRP:HB3	1:A:227:SER:O	2.20	0.40
1:A:219:VAL:HA	1:A:222:ILE:HD12	2.02	0.40
1:C:107:ARG:HG3	1:C:107:ARG:H	1.62	0.40
1:A:233:ASP:HB3	1:A:239:ALA:HB2	2.02	0.40
2:B:119:ARG:HG3	2:B:127:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/355 (99%)	346 (98%)	6 (2%)	0	100	100
1	C	355/355 (100%)	339 (96%)	15 (4%)	1 (0%)	41	50
2	B	321/332 (97%)	315 (98%)	6 (2%)	0	100	100
2	D	338/332 (102%)	329 (97%)	9 (3%)	0	100	100
All	All	1366/1374 (99%)	1329 (97%)	36 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	282	LEU

### 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	305/303 (101%)	286 (94%)	19 (6%)	18	25
1	C	308/303 (102%)	294 (96%)	14 (4%)	27	39
2	B	273/282 (97%)	261 (96%)	12 (4%)	28	39
2	D	290/282 (103%)	273 (94%)	17 (6%)	19	27
All	All	1176/1170 (100%)	1114 (95%)	62 (5%)	24	31

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	47	THR
1	A	54	ASN
1	A	123	ASN
1	A	131	TRP
1	A	175[A]	GLU
1	A	175[B]	GLU
1	A	205	LEU
1	A	260	ILE
1	A	262	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	266	GLN
1	A	283	LYS
1	A	290	ARG
1	A	291	ARG
1	A	292	ILE
1	A	293	ASP
1	A	310	ILE
1	A	346	ASP
1	A	353	GLU
2	B	1	MET
2	B	13	SER
2	B	18	ASP
2	B	37	ASP
2	B	173	ASN
2	B	193	ARG
2	B	213	GLN
2	B	231	ASN
2	B	233	ASN
2	B	258	THR
2	B	262	GLN
2	B	318	ASN
1	C	9	THR
1	C	10[A]	TYR
1	C	10[B]	TYR
1	C	29	LYS
1	C	54	ASN
1	C	89	ASP
1	C	107	ARG
1	C	131	TRP
1	C	229	ILE
1	C	260	ILE
1	C	276	GLN
1	C	281	VAL
1	C	282	LEU
1	C	353	GLU
2	D	14	LYS
2	D	18	ASP
2	D	33[A]	GLN
2	D	33[B]	GLN
2	D	70[A]	LYS
2	D	70[B]	LYS
2	D	122[A]	ASP

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Mol	Chain	Res	Type
2	D	122[B]	ASP
2	D	123	SER
2	D	173	ASN
2	D	213	GLN
2	D	225	LYS
2	D	231	ASN
2	D	233	ASN
2	D	244	ARG
2	D	258	THR
2	D	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	70	ASN
1	A	123	ASN
1	A	140	ASN
1	A	204	GLN
1	A	215	HIS
1	A	234	HIS
1	A	245	ASN
1	A	249	HIS
1	A	313	GLN
1	A	344	GLN
2	B	9	ASN
2	B	49	ASN
2	B	95	GLN
2	B	124	GLN
2	B	136	ASN
2	B	173	ASN
2	B	209	HIS
2	B	213	GLN
2	B	231	ASN
2	B	232	GLN
2	B	233	ASN
2	B	262	GLN
2	B	307	GLN
1	C	26	ASN
1	C	70	ASN
1	C	123	ASN
1	C	140	ASN

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Mol	Chain	Res	Type
1	C	204	GLN
1	C	237	ASN
1	C	256	ASN
1	C	313	GLN
1	C	322	ASN
2	D	49	ASN
2	D	95	GLN
2	D	124	GLN
2	D	136	ASN
2	D	173	ASN
2	D	231	ASN
2	D	232	GLN
2	D	233	ASN
2	D	257	ASN
2	D	281	GLN
2	D	307	GLN
2	D	318	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

19 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
5	SO4	A	360	-	4,4,4	0.30	0	6,6,6	0.41	0
5	SO4	A	359	-	4,4,4	0.27	0	6,6,6	0.22	0
3	FMN	A	3402[A]	-	33,33,33	1.30	2 (6%)	48,50,50	1.63	11 (22%)
4	PO4	A	356[B]	-	4,4,4	3.91	4 (100%)	6,6,6	0.91	0
5	SO4	D	337	-	4,4,4	0.25	0	6,6,6	0.64	0
5	SO4	B	333	-	4,4,4	0.14	0	6,6,6	0.70	0
4	PO4	C	359	-	4,4,4	1.39	0	6,6,6	1.78	2 (33%)
5	SO4	D	334	-	4,4,4	0.17	0	6,6,6	0.41	0
5	SO4	A	361	-	4,4,4	0.24	0	6,6,6	0.44	0
5	SO4	C	357	-	4,4,4	0.24	0	6,6,6	0.51	0
5	SO4	A	357	-	4,4,4	0.24	0	6,6,6	0.85	0
5	SO4	B	335	-	4,4,4	0.30	0	6,6,6	0.68	0
5	SO4	D	335	-	4,4,4	0.41	0	6,6,6	0.77	0
5	SO4	C	358	-	4,4,4	0.13	0	6,6,6	0.43	0
5	SO4	B	334	-	4,4,4	0.47	0	6,6,6	0.61	0
5	SO4	D	336	-	4,4,4	0.33	0	6,6,6	0.81	0
5	SO4	A	358	-	4,4,4	0.31	0	6,6,6	0.66	0
5	SO4	D	333	-	4,4,4	0.15	0	6,6,6	0.48	0
5	SO4	C	356	-	4,4,4	0.17	0	6,6,6	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	A	3402[A]	-	-	8/18/18/18	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3402[A]	FMN	C4A-N5	4.62	1.39	1.30
4	A	356[B]	PO4	P-O2	-4.49	1.41	1.54
4	A	356[B]	PO4	P-O3	-4.40	1.41	1.54
4	A	356[B]	PO4	P-O4	-3.88	1.42	1.54
4	A	356[B]	PO4	P-O1	-2.55	1.44	1.50
3	A	3402[A]	FMN	C10-N1	2.47	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3402[A]	FMN	C4'-C3'-C2'	3.34	120.31	113.36
3	A	3402[A]	FMN	C10-N1-C2	3.09	123.09	116.90
3	A	3402[A]	FMN	C4A-C10-N1	-3.08	117.58	124.73
3	A	3402[A]	FMN	C4A-C4-N3	3.03	120.89	113.19
3	A	3402[A]	FMN	C4A-C10-N10	3.01	120.88	116.48
3	A	3402[A]	FMN	C4-N3-C2	-3.00	120.09	125.64
3	A	3402[A]	FMN	C10-C4A-N5	-2.82	118.86	124.86
4	C	359	PO4	O4-P-O2	2.75	116.81	107.97
4	C	359	PO4	O4-P-O1	-2.44	101.96	110.89
3	A	3402[A]	FMN	C9A-C5A-N5	-2.29	119.95	122.43
3	A	3402[A]	FMN	C5A-N5-C4A	2.26	121.83	118.07
3	A	3402[A]	FMN	C4-C4A-N5	2.17	121.33	118.23
3	A	3402[A]	FMN	O3'-C3'-C4'	-2.15	103.63	108.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3402[A]	FMN	C2'-C3'-C4'-C5'
3	A	3402[A]	FMN	C3'-C4'-C5'-O5'
3	A	3402[A]	FMN	C5'-O5'-P-O1P
3	A	3402[A]	FMN	C5'-O5'-P-O2P
3	A	3402[A]	FMN	O3'-C3'-C4'-C5'
3	A	3402[A]	FMN	O3'-C3'-C4'-O4'
3	A	3402[A]	FMN	C2'-C3'-C4'-O4'
3	A	3402[A]	FMN	C5'-O5'-P-O3P

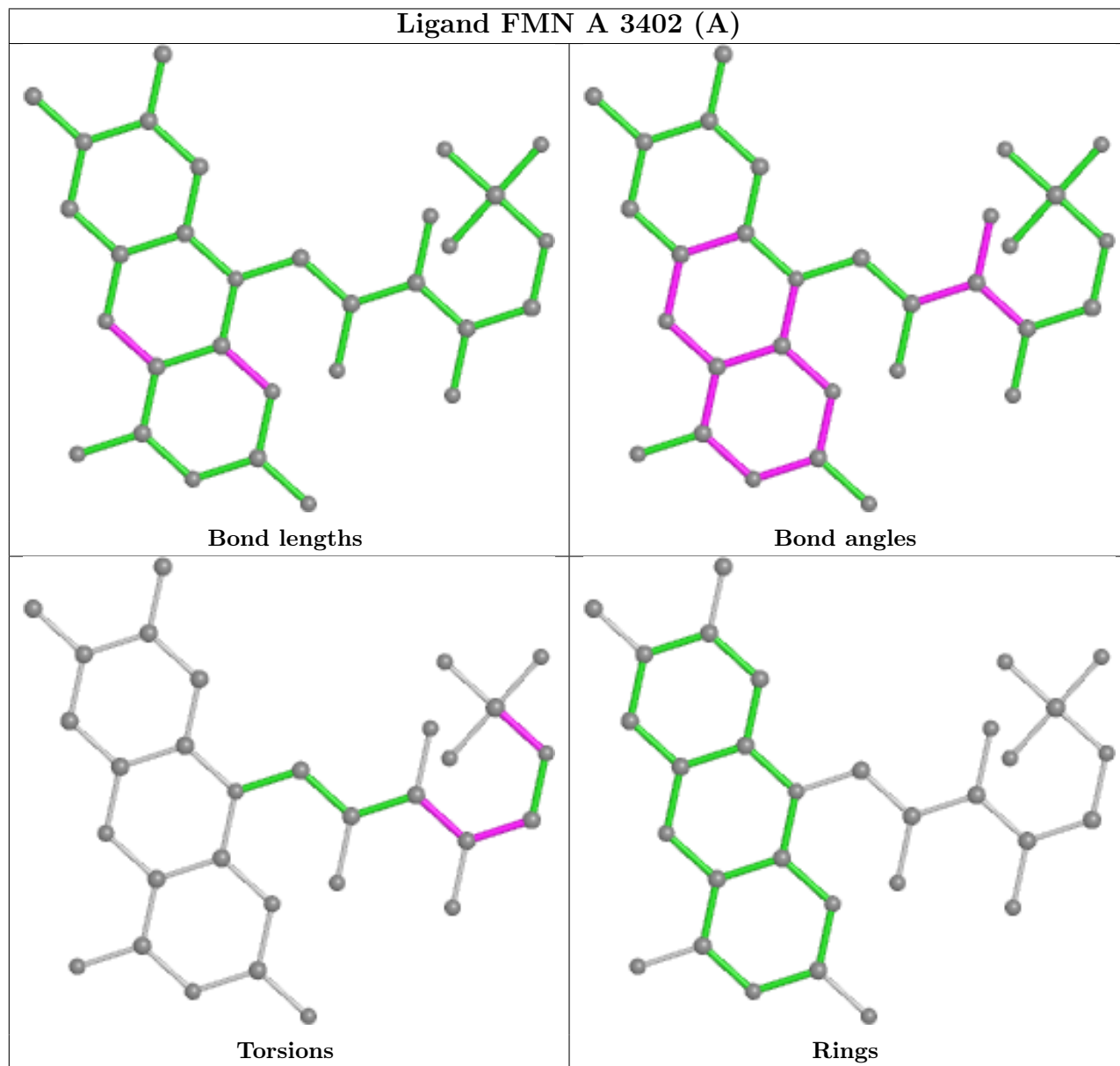
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3402[A]	FMN	1	0
4	A	356[B]	PO4	1	0
4	C	359	PO4	2	0
5	A	361	SO4	2	0
5	B	335	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	349/355 (98%)	-0.49	7 (2%) 65 71	11, 20, 36, 66	0
1	C	348/355 (98%)	-0.10	11 (3%) 47 54	17, 33, 56, 79	0
2	B	318/332 (95%)	-0.48	4 (1%) 77 81	10, 21, 36, 49	0
2	D	325/332 (97%)	-0.50	2 (0%) 89 92	15, 24, 39, 42	0
All	All	1340/1374 (97%)	-0.39	24 (1%) 68 74	10, 24, 45, 79	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	355	GLN	7.3
1	A	175[A]	GLU	4.5
2	B	258	THR	4.1
2	B	257	ASN	3.9
1	C	283	LYS	3.8
1	C	265	ASP	3.7
2	B	256	SER	3.6
1	C	281	VAL	3.5
1	A	355	GLN	3.4
1	C	282	LEU	3.3
1	A	265	ASP	3.2
1	C	109	LEU	2.9
1	C	263	ASP	2.8
1	C	214	GLU	2.7
1	A	291	ARG	2.7
1	A	263	ASP	2.7
2	D	122[A]	ASP	2.7
1	C	165	GLN	2.7
1	C	122	ASP	2.6
1	C	216	GLY	2.5
2	B	122[A]	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	290	ARG	2.4
1	A	283	LYS	2.2
2	D	256	SER	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](#)

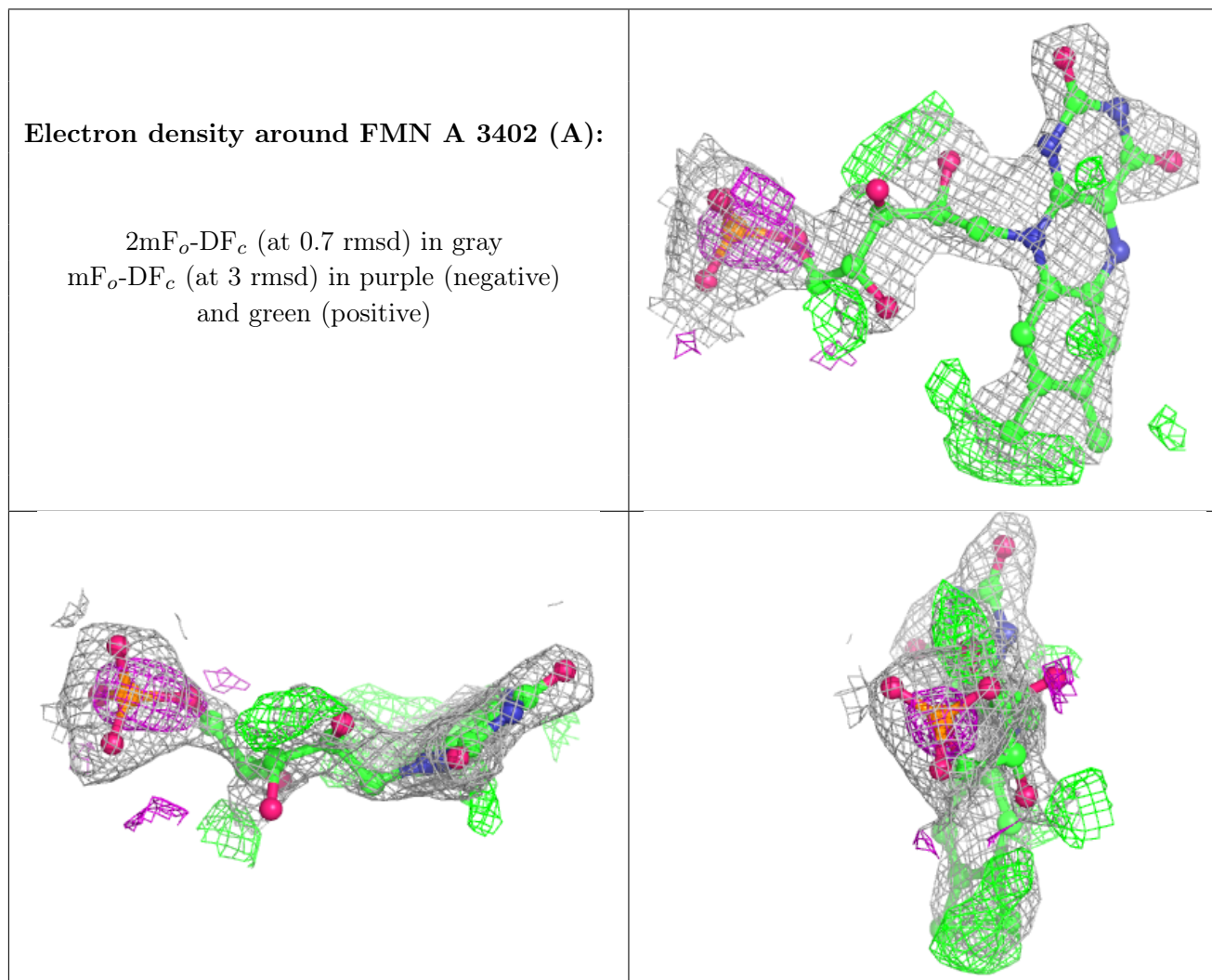
There are no monosaccharides in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
5	SO4	B	335	5/5	0.82	0.20	47,50,52,52	5
5	SO4	C	357	5/5	0.86	0.18	49,50,53,53	5
5	SO4	D	336	5/5	0.86	0.19	23,23,27,27	5
3	FMN	A	3402[A]	31/31	0.89	0.28	18,26,33,35	31
5	SO4	D	335	5/5	0.90	0.20	41,47,51,51	0
5	SO4	B	334	5/5	0.91	0.25	53,55,57,59	0
5	SO4	A	361	5/5	0.95	0.19	25,28,30,32	5
5	SO4	D	334	5/5	0.95	0.23	56,58,60,60	0
5	SO4	D	333	5/5	0.96	0.17	58,59,61,62	0
5	SO4	C	356	5/5	0.96	0.21	63,63,64,66	0
5	SO4	D	337	5/5	0.96	0.12	33,33,35,35	5
4	PO4	C	359	5/5	0.97	0.13	32,33,35,38	5
5	SO4	A	358	5/5	0.97	0.10	21,22,24,25	5
5	SO4	C	358	5/5	0.97	0.18	64,67,67,67	0
5	SO4	A	360	5/5	0.97	0.10	55,55,58,59	0
5	SO4	A	357	5/5	0.98	0.14	41,42,44,46	0
5	SO4	A	359	5/5	0.98	0.12	48,49,52,53	0
4	PO4	A	356[B]	5/5	0.99	0.18	20,20,20,20	5
5	SO4	B	333	5/5	0.99	0.12	35,38,40,40	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.