



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 11:01 AM BST

PDB ID : 5G5G  
Title : Escherichia coli Periplasmic Aldehyde Oxidase  
Authors : Correia, M.A.S.; Otrelo-Cardoso, A.R.; Romao, M.J.; Santos-Silva, T.  
Deposited on : 2016-05-25  
Resolution : 1.70 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.

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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 : 2.13.1  
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) : 2.13.1

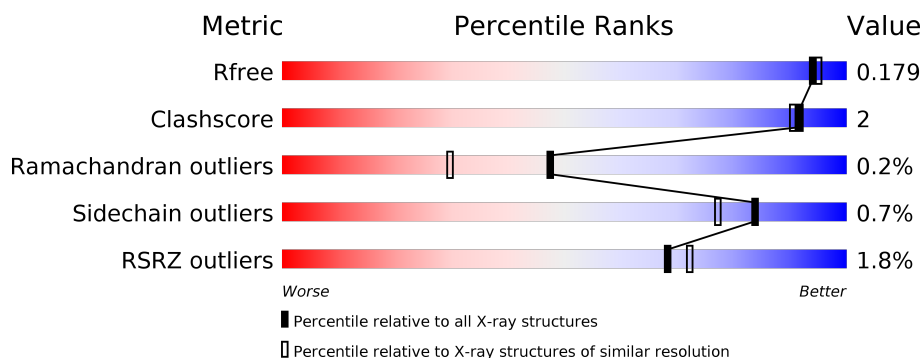
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	229	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 73%; width: 27%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 73%; width: 27%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 73%; width: 27%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 0; left: 73%; width: 27%; height: 10px; background-color: red;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>73%</span> <span>24%</span> </div> </div>
2	B	318	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 94%; width: 6%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 94%; width: 6%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 94%; width: 6%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 0; left: 94%; width: 6%; height: 10px; background-color: red;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>94%</span> <span>5%</span> </div> </div>
3	C	732	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 95%; width: 5%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 95%; width: 5%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 95%; width: 5%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 0; left: 95%; width: 5%; height: 10px; background-color: red;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>95%</span> <span>.</span> </div> </div>

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	CL	A	1229	-	-	X	-
7	ACT	B	1321	-	-	X	-
9	SF4	B	320	-	-	X	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10479 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 PUTATIVE XANTHINE DEHYDROGENASE YAGT IRON-SULFUR-BINDING SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	7	0
			1341	820	239	269	13			

- Molecule 2 is a protein called PUTATIVE XANTHINE DEHYDROGENASE YAGR MOLYBDENUM-BINDING SU SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	316	Total	C	N	O	S	0	4	0
			2400	1509	439	444	8			

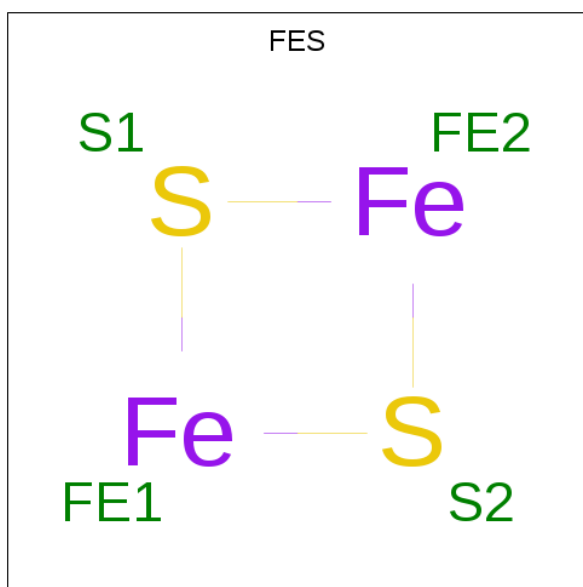
- Molecule 3 is a protein called PUTATIVE XANTHINE DEHYDROGENASE YAGS FAD-BINDING SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	731	Total	C	N	O	S	0	14	0
			5569	3477	989	1076	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	VAL	ALA	cloning artifact	UNP P77489
C	391	GLY	ASP	cloning artifact	UNP P77489

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		

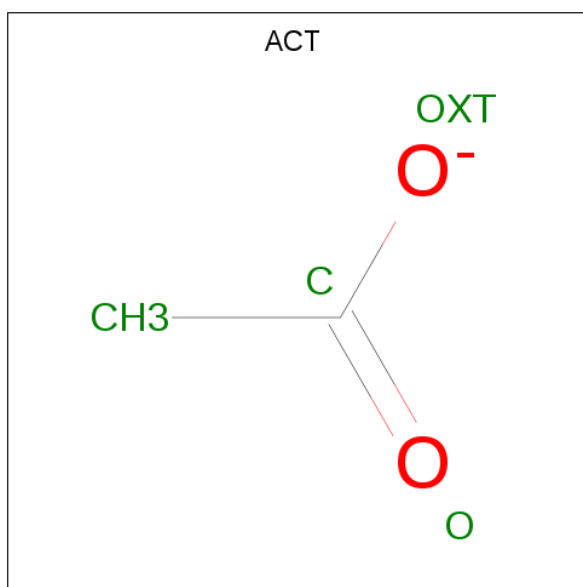
- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	I	0	0
			2	2		
5	A	2	Total	I	0	0
			2	2		
5	C	3	Total	I	0	0
			3	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

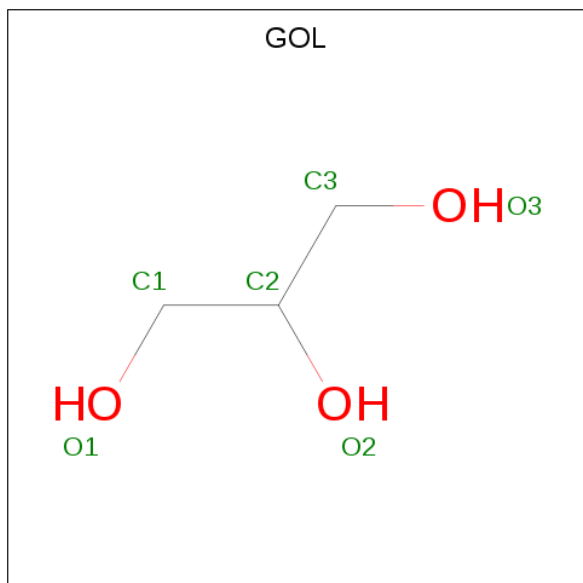
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Cl	0	0
			4	4		
6	A	3	Total	Cl	0	0
			3	3		
6	C	5	Total	Cl	0	0
			5	5		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



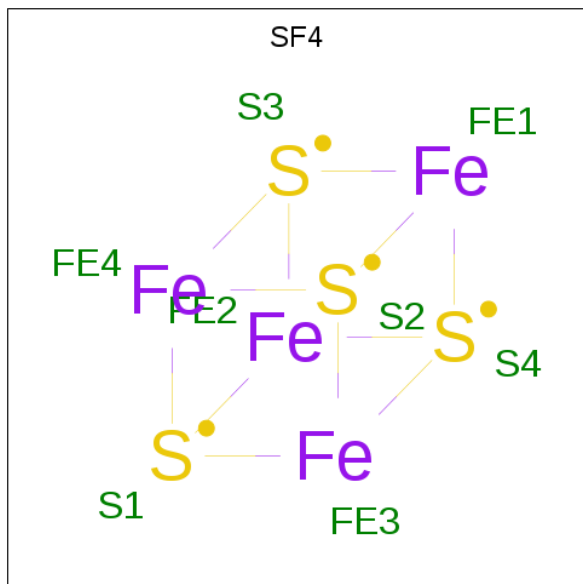
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



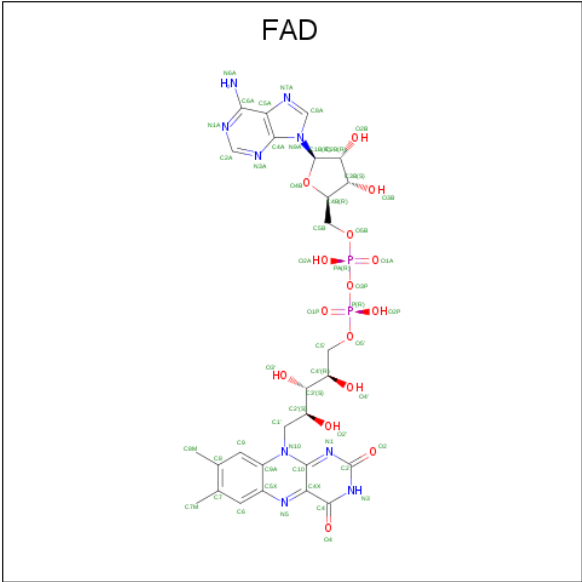
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



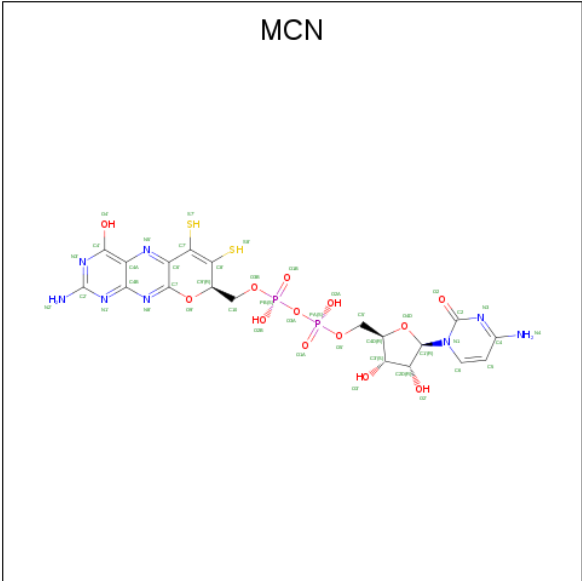
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

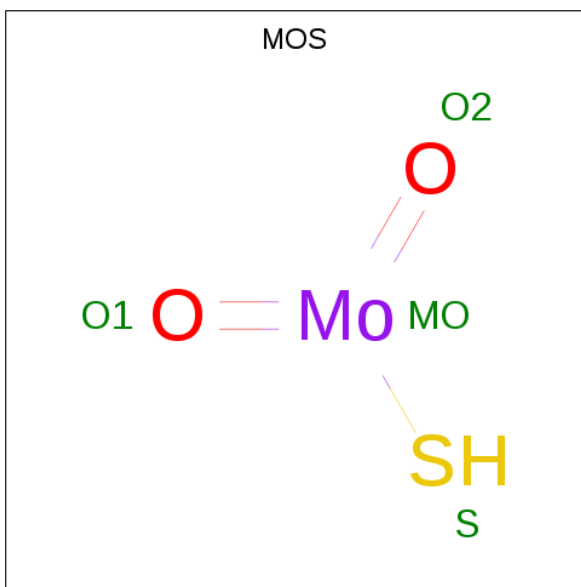
- Molecule 11 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula:  $C_{19}H_{22}N_8O_{13}P_2S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O	P	0	0
			44	19	8	13	2		

- Molecule 12 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $HMoO_2S$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	Mo	O	S	0	0
			4	1	2	1		

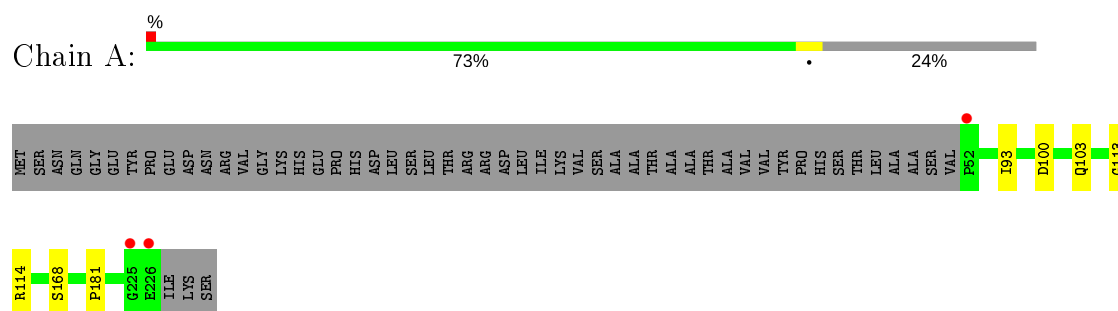
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	175	Total	O	0	0
			175	175		
13	B	248	Total	O	0	0
			248	248		
13	C	558	Total	O	0	0
			558	558		

### 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: PUTATIVE XANTHINE DEHYDROGENASE YAGT IRON-SULFUR-BINDING SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.68Å 78.34Å 151.91Å 90.00° 99.69° 90.00°	Depositor
Resolution (Å)	48.32 – 1.70 48.32 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.32-1.70) 98.5 (48.32-1.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.138 , 0.167 0.153 , 0.179	Depositor DCC
$R_{free}$ test set	6835 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10479	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: GOL, MCN, CL, MOS, CSD, SF4, FES, ACT, IOD, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.72	0/1364	0.82	2/1850 (0.1%)
2	B	0.70	0/2447	0.84	8/3327 (0.2%)
3	C	0.77	1/5693 (0.0%)	0.88	9/7730 (0.1%)
All	All	0.75	1/9504 (0.0%)	0.86	19/12907 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	84	SER	CB-OG	-6.53	1.33	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH2	-8.36	116.12	120.30
3	C	417	ARG	NE-CZ-NH1	8.24	124.42	120.30
3	C	450	ARG	NE-CZ-NH1	7.27	123.94	120.30
2	B	118[A]	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	B	118[B]	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	B	132	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	B	132	ARG	NE-CZ-NH1	6.55	123.58	120.30
3	C	260	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	114	ARG	NE-CZ-NH1	5.78	123.19	120.30
3	C	537	ASP	CB-CG-OD1	5.77	123.49	118.30
2	B	118[A]	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	B	118[B]	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	B	83	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	B	83	ARG	NE-CZ-NH1	5.41	123.00	120.30
3	C	264	ARG	NE-CZ-NH2	-5.40	117.60	120.30
3	C	417	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	C	294	ASP	CB-CG-OD1	5.24	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	98	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	C	69	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1341	0	1319	4	0
2	B	2400	0	2449	13	0
3	C	5569	0	5522	14	0
4	A	8	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	1	0
6	A	3	0	0	3	0
6	B	4	0	0	0	0
6	C	5	0	0	0	0
7	A	4	0	3	0	0
7	B	4	0	3	3	0
7	C	8	0	6	0	0
8	A	12	0	16	1	0
8	B	12	0	16	1	0
8	C	12	0	16	1	0
9	B	8	0	0	3	0
10	B	53	0	31	0	0
11	C	44	0	16	0	0
12	C	4	0	0	0	0
13	A	175	0	0	0	1
13	B	248	0	0	0	0
13	C	558	0	0	0	1
All	All	10479	0	9397	30	1

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 2.

All (30) 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:B:129:CYS:HG	9:B:320:SF4:FE2	0.63	0.91
1:A:103:GLN:OE1	6:A:1229:CL:CL	2.30	0.86
3:C:53[A]:ILE:HD11	3:C:254:LEU:HD12	1.73	0.70
2:B:157:CYS:HG	9:B:320:SF4:FE4	1.11	0.68
3:C:25:ILE:HD12	8:C:1742:GOL:H31	1.79	0.65
3:C:53[A]:ILE:HD11	3:C:254:LEU:CD1	2.28	0.63
2:B:157:CYS:SG	9:B:320:SF4:FE4	1.90	0.63
2:B:64:ALA:H	7:B:1321:ACT:H3	1.65	0.62
3:C:65:ALA:HB3	3:C:133[B]:HIS:CD2	2.36	0.61
6:A:1229:CL:CL	3:C:655:ASP:HB2	2.41	0.57
2:B:62:THR:HB	7:B:1321:ACT:H1	1.89	0.55
3:C:53[B]:ILE:HD12	3:C:270:LEU:CD2	2.39	0.52
2:B:20:GLN:HB2	2:B:181:PRO:HB3	1.90	0.51
3:C:556:THR:HG22	3:C:559:GLU:HG3	1.92	0.50
2:B:275:LEU:HD22	2:B:311:LEU:HD21	1.93	0.50
3:C:137[B]:ASN:OD1	3:C:138:LYS:N	2.44	0.50
2:B:251[B]:ASP:C	2:B:251[B]:ASP:OD1	2.49	0.48
3:C:53[B]:ILE:HD12	3:C:270:LEU:HD22	1.96	0.47
2:B:64:ALA:N	7:B:1321:ACT:H3	2.28	0.47
3:C:359:MET:HG2	3:C:699:SER:HB2	1.95	0.47
2:B:268:ILE:HG12	8:B:1322:GOL:C1	2.45	0.47
2:B:118[B]:ARG:HD2	2:B:118[B]:ARG:HA	1.43	0.43
1:A:113:GLY:O	6:A:1228:CL:CL	2.73	0.43
3:C:47:ASN:HB2	5:C:1732:IOD:I	2.89	0.43
3:C:585:THR:HB	3:C:693:LEU:HD22	2.00	0.43
1:A:93:ILE:C	1:A:93:ILE:HD12	2.39	0.42
8:A:1232:GOL:H32	2:B:123:TYR:CD1	2.55	0.42
1:A:181:PRO:HG2	2:B:96:LEU:HD11	2.00	0.42
3:C:614:GLY:HA2	3:C:677:ASP:O	2.20	0.42
3:C:198:VAL:HG22	3:C:265:PRO:HB3	2.01	0.41

All (1) 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)
13:A:2030:HOH:O	13:C:2076:HOH:O[3_445]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/229 (79%)	177 (98%)	3 (2%)	0	100	100
2	B	318/318 (100%)	315 (99%)	3 (1%)	0	100	100
3	C	742/732 (101%)	727 (98%)	13 (2%)	2 (0%)	41	24
All	All	1240/1279 (97%)	1219 (98%)	19 (2%)	2 (0%)	47	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	241	GLY
3	C	350	ARG

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	148/186 (80%)	146 (99%)	2 (1%)	67	53
2	B	247/244 (101%)	246 (100%)	1 (0%)	91	87
3	C	578/565 (102%)	573 (99%)	5 (1%)	78	70
All	All	973/995 (98%)	965 (99%)	8 (1%)	84	74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP

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Mol	Chain	Res	Type
1	A	168	SER
2	B	237	TYR
3	C	53[A]	ILE
3	C	53[B]	ILE
3	C	91	LYS
3	C	552	THR
3	C	556	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
3	CSD	C	395	3	3,7,8	0.74	0	1,8,10	6.34	1 (100%)

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	CSD	C	395	3	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	395	CSD	OD1-SG-CB	-6.34	93.47	105.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	395	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 19 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	GOL	C	1741	-	5,5,5	0.54	0	5,5,5	0.69	0
8	GOL	C	1742	-	5,5,5	0.41	0	5,5,5	1.11	0
11	MCN	C	921	12	38,48,48	4.61	18 (47%)	40,74,74	4.84	20 (50%)
9	SF4	B	320	2	0,12,12	0.00	-	-	-	-
10	FAD	B	321	-	51,58,58	3.68	20 (39%)	60,89,89	4.75	26 (43%)
8	GOL	A	1233	-	5,5,5	0.32	0	5,5,5	0.84	0
7	ACT	C	1740	-	1,3,3	1.22	0	0,3,3	0.00	-
7	ACT	C	1739	-	1,3,3	1.75	0	0,3,3	0.00	-
8	GOL	B	1323	-	5,5,5	0.38	0	5,5,5	0.40	0
4	FES	A	231	1	0,4,4	0.00	-	-	-	-
8	GOL	A	1232	-	5,5,5	0.47	0	5,5,5	0.93	0
12	MOS	C	922	11	0,3,3	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ACT	B	1321	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
8	GOL	B	1322	-	5,5,5	0.54	0	5,5,5	0.39	0
7	ACT	A	1231	-	1,3,3	0.70	0	0,3,3	0.00	-
4	FES	A	230	1	0,4,4	0.00	-	-		

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
8	GOL	C	1741	-	-	0/4/4/4	-
11	MCN	C	921	12	-	2/20/54/54	0/5/5/5
9	SF4	B	320	2	-	-	0/6/5/5
10	FAD	B	321	-	-	0/30/50/50	0/6/6/6
8	GOL	A	1233	-	-	2/4/4/4	-
8	GOL	B	1322	-	-	1/4/4/4	-
8	GOL	B	1323	-	-	0/4/4/4	-
4	FES	A	231	1	-	-	0/1/1/1
8	GOL	A	1232	-	-	3/4/4/4	-
8	GOL	C	1742	-	-	2/4/4/4	-
4	FES	A	230	1	-	-	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	921	MCN	C6'-N5'	16.37	1.56	1.32
10	B	321	FAD	C2A-N3A	12.35	1.52	1.32
11	C	921	MCN	C6'-C7	11.59	1.60	1.43
10	B	321	FAD	C4X-N5	10.64	1.48	1.33
11	C	921	MCN	C4A-C4B	9.48	1.57	1.40
11	C	921	MCN	C2-N3	7.60	1.53	1.38
10	B	321	FAD	C2B-C1B	-7.39	1.42	1.53
11	C	921	MCN	C7-N8'	7.23	1.48	1.30
10	B	321	FAD	C10-N1	6.84	1.42	1.33
11	C	921	MCN	C4A-N5'	6.61	1.50	1.37
10	B	321	FAD	C9-C8	5.72	1.52	1.37
10	B	321	FAD	C5'-C4'	5.69	1.59	1.51
10	B	321	FAD	C9A-N10	5.42	1.45	1.38
11	C	921	MCN	O9'-C9'	-5.40	1.33	1.44
10	B	321	FAD	O4B-C1B	5.33	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	321	FAD	O3'-C3'	4.90	1.54	1.43
10	B	321	FAD	O4B-C4B	4.76	1.55	1.45
10	B	321	FAD	C4'-C3'	-4.57	1.44	1.53
11	C	921	MCN	C2'-N2'	-4.46	1.25	1.33
10	B	321	FAD	C8M-C8	-4.12	1.42	1.51
10	B	321	FAD	C2A-N1A	-4.11	1.26	1.33
11	C	921	MCN	C5-C4	4.00	1.50	1.41
10	B	321	FAD	C2'-C3'	-3.74	1.46	1.53
10	B	321	FAD	C9A-C5X	3.69	1.50	1.42
11	C	921	MCN	C6-C5	-3.43	1.30	1.38
11	C	921	MCN	C5'-C4D	-3.14	1.41	1.51
11	C	921	MCN	C3'-C2D	-3.12	1.44	1.53
10	B	321	FAD	C2-N1	-3.05	1.32	1.38
10	B	321	FAD	C3B-C4B	-3.01	1.45	1.53
11	C	921	MCN	O4D-C4D	2.82	1.51	1.45
11	C	921	MCN	C2D-C1'	2.73	1.57	1.53
11	C	921	MCN	C3'-C4D	2.73	1.60	1.53
10	B	321	FAD	O2'-C2'	2.68	1.49	1.43
10	B	321	FAD	C1'-N10	2.53	1.50	1.48
7	B	1321	ACT	CH3-C	-2.37	1.45	1.48
10	B	321	FAD	C4A-N3A	-2.35	1.32	1.35
11	C	921	MCN	C4-N4	-2.08	1.29	1.35
11	C	921	MCN	C10-C9'	-2.07	1.49	1.52
11	C	921	MCN	O3'-C3'	2.04	1.47	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	321	FAD	C4-N3-C2	22.76	134.36	115.14
11	C	921	MCN	C2-N3-C4	16.76	133.32	116.34
10	B	321	FAD	C2A-N1A-C6A	11.84	139.01	118.75
10	B	321	FAD	N3A-C2A-N1A	-11.42	110.83	128.68
10	B	321	FAD	C4X-C4-N3	-10.03	109.71	123.43
11	C	921	MCN	N1'-C2'-N3'	-9.64	114.37	127.22
11	C	921	MCN	C4B-C4A-N5'	-9.54	110.90	122.41
10	B	321	FAD	C4A-C5A-N7A	8.89	118.67	109.40
11	C	921	MCN	C5-C4-N3	-8.34	112.10	121.72
11	C	921	MCN	N4-C4-N3	7.97	129.09	116.49
11	C	921	MCN	O9'-C7-N8'	-7.63	105.83	115.30
11	C	921	MCN	O4'-C4'-N3'	6.62	134.88	117.44
11	C	921	MCN	C2'-N1'-C4B	6.29	122.54	115.36
10	B	321	FAD	C1'-N10-C9A	5.66	122.75	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	921	MCN	C2'-N3'-C4'	5.66	130.69	116.43
10	B	321	FAD	C8M-C8-C7	5.63	132.28	120.74
10	B	321	FAD	C6-C7-C8	5.45	129.09	119.91
11	C	921	MCN	O4D-C4D-C3'	-5.14	94.94	105.11
10	B	321	FAD	C5A-C6A-N1A	-4.96	109.11	120.35
10	B	321	FAD	C4X-C10-N10	4.89	125.32	120.30
10	B	321	FAD	C7M-C7-C8	-4.74	111.03	120.74
11	C	921	MCN	C2D-C3'-C4D	4.49	111.36	102.64
10	B	321	FAD	C6-C5X-C9A	-4.45	113.22	119.05
10	B	321	FAD	C1B-N9A-C4A	4.43	134.43	126.64
11	C	921	MCN	O4'-C4'-C4A	-4.39	111.46	119.67
11	C	921	MCN	C7-N8'-C4B	4.33	120.30	116.61
10	B	321	FAD	O4B-C4B-C5B	-4.18	95.63	109.37
10	B	321	FAD	N6A-C6A-N1A	4.11	127.10	118.57
11	C	921	MCN	C4A-C4B-N1'	-3.74	115.65	121.71
10	B	321	FAD	C8M-C8-C9	-3.64	111.64	120.34
10	B	321	FAD	C10-C4X-N5	-3.48	118.85	121.26
10	B	321	FAD	C5X-C9A-N10	-3.32	115.31	117.72
10	B	321	FAD	C9-C8-C7	-3.30	114.36	119.91
10	B	321	FAD	C9-C9A-C5X	3.28	125.48	119.88
11	C	921	MCN	C6-N1-C2	3.26	126.38	121.20
10	B	321	FAD	C9A-N10-C10	-3.25	117.65	121.91
11	C	921	MCN	N2'-C2'-N1'	3.20	123.00	117.79
10	B	321	FAD	O3B-C3B-C4B	-3.19	101.81	111.05
10	B	321	FAD	C2B-C3B-C4B	3.00	108.47	102.64
10	B	321	FAD	C4-C4X-C10	2.73	121.76	119.95
11	C	921	MCN	PB-O3A-PA	-2.66	123.68	132.83
11	C	921	MCN	C5'-C4D-C3'	2.58	124.84	115.18
10	B	321	FAD	C5A-C6A-N6A	2.26	123.79	120.35
11	C	921	MCN	O3'-C3'-C4D	-2.17	104.78	111.05
10	B	321	FAD	C9A-C5X-N5	2.13	125.70	122.36
11	C	921	MCN	O3'-C3'-C2D	2.06	118.47	111.82

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1232	GOL	O1-C1-C2-C3
8	A	1233	GOL	O1-C1-C2-C3
8	A	1232	GOL	O1-C1-C2-O2
8	A	1233	GOL	O1-C1-C2-O2
11	C	921	MCN	C3'-C4D-C5'-O5'

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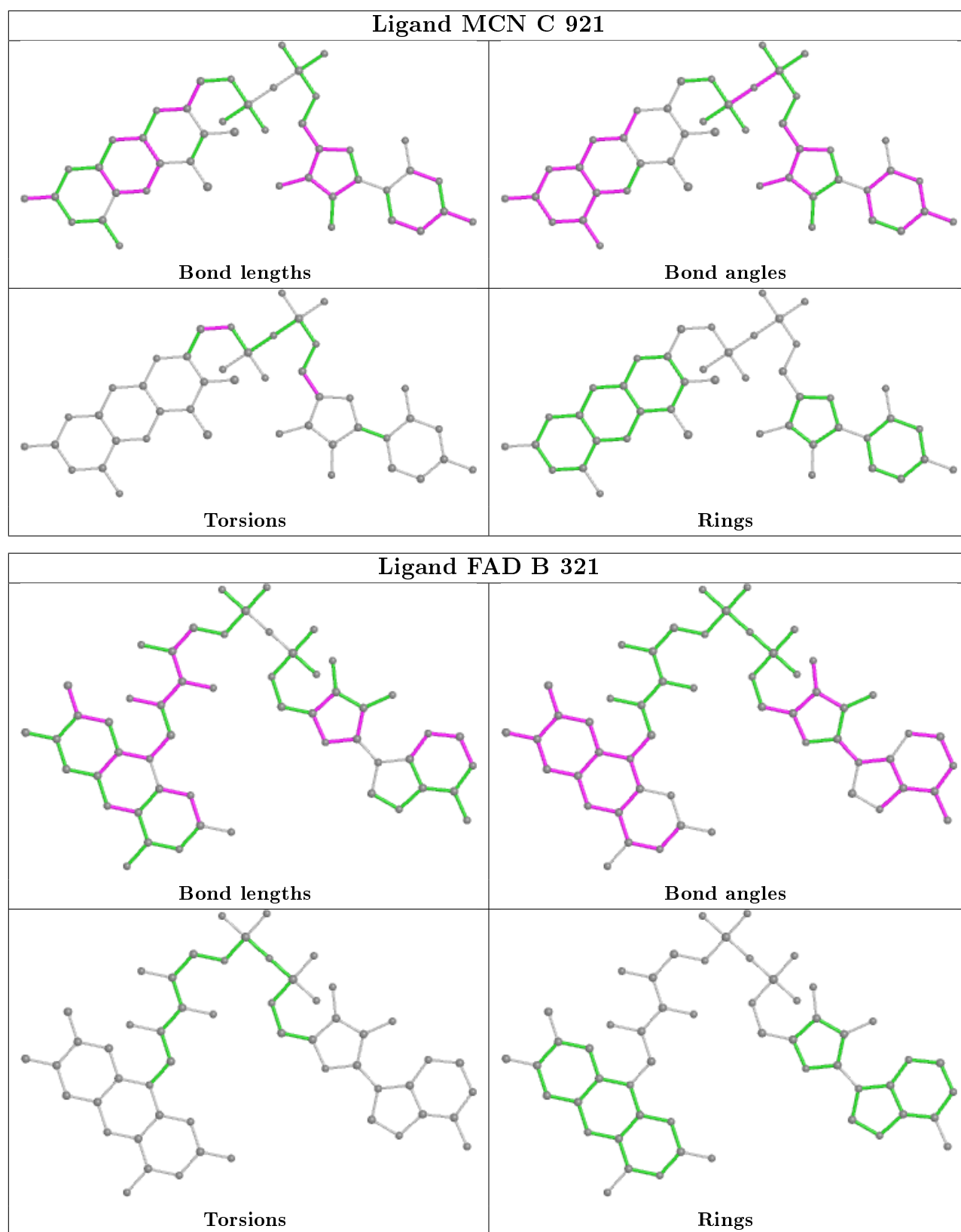
Mol	Chain	Res	Type	Atoms
11	C	921	MCN	C9'-C10-O3B-PB
8	C	1742	GOL	O2-C2-C3-O3
8	B	1322	GOL	O1-C1-C2-C3
8	C	1742	GOL	C1-C2-C3-O3
8	A	1232	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1742	GOL	1	0
9	B	320	SF4	3	0
8	A	1232	GOL	1	0
7	B	1321	ACT	3	0
8	B	1322	GOL	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 ⓘ

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	175/229 (76%)	-0.26	3 (1%) 70 74	10, 16, 31, 60	0
2	B	316/318 (99%)	-0.19	7 (2%) 62 66	11, 21, 36, 62	0
3	C	730/732 (99%)	-0.31	12 (1%) 72 76	10, 17, 35, 61	0
All	All	1221/1279 (95%)	-0.27	22 (1%) 68 72	10, 17, 35, 62	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	731	VAL	4.3
3	C	562	ALA	3.8
3	C	551	GLY	3.8
1	A	52	PRO	3.8
3	C	730	ASP	3.6
3	C	558	HIS	3.5
1	A	226	GLU	3.4
2	B	181	PRO	3.4
2	B	23	PRO	3.2
1	A	225	GLY	3.2
2	B	182	GLU	3.1
2	B	21	ARG	3.1
3	C	64	THR	3.0
3	C	563	GLY	3.0
3	C	550	ASN	2.9
3	C	155	GLU	2.8
3	C	552	THR	2.7
3	C	553	ARG	2.6
3	C	729	PRO	2.6
2	B	20	GLN	2.2
2	B	17	LEU	2.0
2	B	315	ARG	2.0



## 6.2 Non-standard residues in protein, DNA, RNA chains [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
3	CSD	C	395	8/9	0.97	0.10	17,20,26,27	0

## 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
8	GOL	A	1233	6/6	0.74	0.18	35,40,42,46	0
8	GOL	C	1742	6/6	0.81	0.14	34,39,41,43	0
7	ACT	C	1739	4/4	0.82	0.17	53,53,58,58	0
9	SF4	B	320	8/8	0.84	0.15	15,17,19,20	0
8	GOL	C	1741	6/6	0.86	0.13	28,39,43,43	0
8	GOL	A	1232	6/6	0.88	0.13	26,31,32,40	0
8	GOL	B	1322	6/6	0.90	0.19	39,41,43,45	0
6	CL	A	1230	1/1	0.90	0.07	43,43,43,43	0
7	ACT	B	1321	4/4	0.90	0.18	20,23,34,38	0
7	ACT	A	1231	4/4	0.91	0.09	27,33,34,36	0
6	CL	C	1737	1/1	0.91	0.11	36,36,36,36	0
6	CL	B	4000	1/1	0.93	0.08	29,29,29,29	0
7	ACT	C	1740	4/4	0.93	0.08	34,37,38,39	0
5	IOD	A	3000	1/1	0.94	0.06	30,30,30,30	1
6	CL	B	1319	1/1	0.94	0.07	39,39,39,39	0
8	GOL	B	1323	6/6	0.94	0.14	21,37,40,42	0
6	CL	B	1320	1/1	0.94	0.06	37,37,37,37	0
4	FES	A	230	4/4	0.94	0.11	10,10,11,11	0
6	CL	C	1735	1/1	0.96	0.06	24,24,24,24	0
6	CL	C	4000	1/1	0.97	0.10	26,26,26,26	0
6	CL	A	1229	1/1	0.97	0.10	27,27,27,27	0

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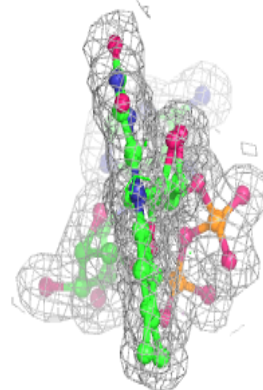
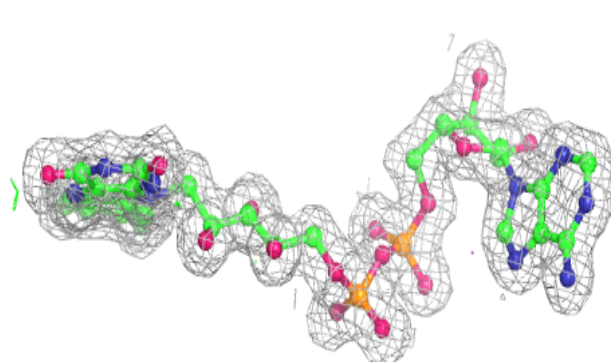
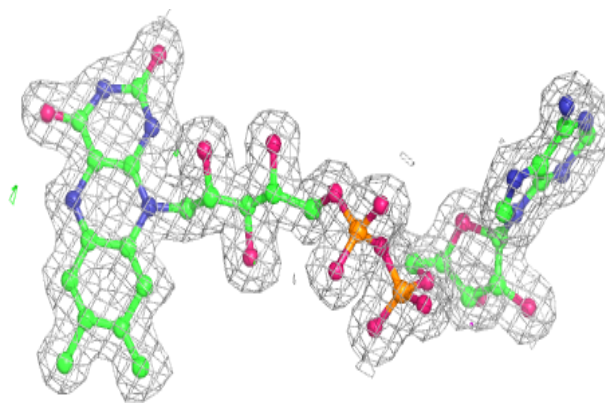
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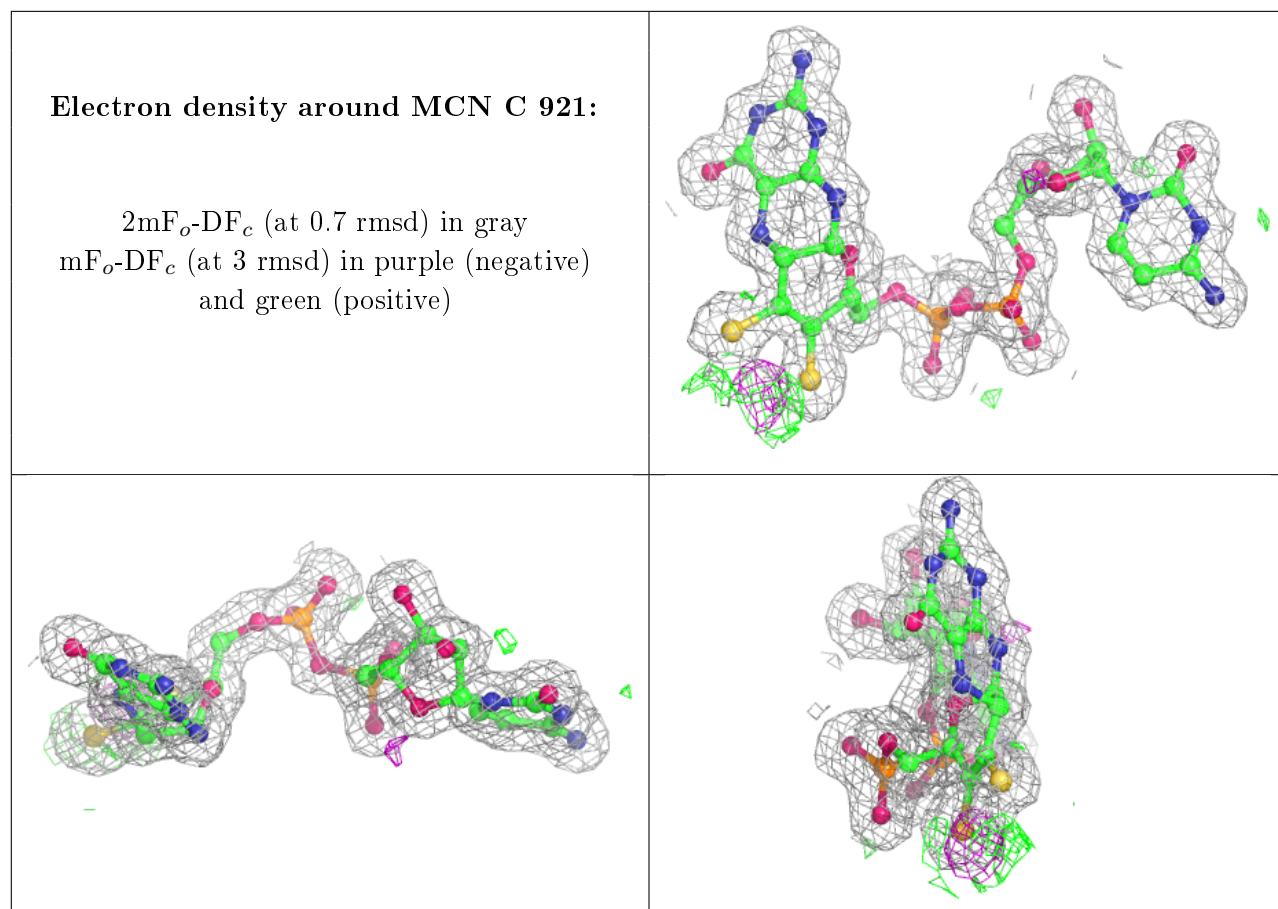
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	IOD	B	1317	1/1	0.98	0.04	28,28,28,28	1
6	CL	C	1736	1/1	0.98	0.05	37,37,37,37	0
10	FAD	B	321	53/53	0.98	0.07	10,12,14,14	0
5	IOD	B	3000	1/1	0.98	0.04	30,30,30,30	1
12	MOS	C	922	4/4	0.99	0.08	12,12,14,14	1
5	IOD	C	1732	1/1	0.99	0.04	23,23,23,23	1
6	CL	B	1318	1/1	0.99	0.06	25,25,25,25	0
11	MCN	C	921	44/44	0.99	0.07	9,10,11,11	0
6	CL	A	1228	1/1	0.99	0.04	29,29,29,29	0
5	IOD	C	1734	1/1	0.99	0.04	27,27,27,27	1
5	IOD	A	1227	1/1	1.00	0.05	13,13,13,13	1
6	CL	C	1738	1/1	1.00	0.04	33,33,33,33	0
5	IOD	C	1733	1/1	1.00	0.03	25,25,25,25	1
4	FES	A	231	4/4	1.00	0.06	9,9,10,10	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 FAD B 321:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.