



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:50 PM GMT

PDB ID : 5BPS  
Title : Structure of the yeast F1FO ATPase C10 ring with oligomycin A  
Authors : Symersky, J.; Xu, T.; Mueller, D.M.  
Deposited on : 2015-05-28  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

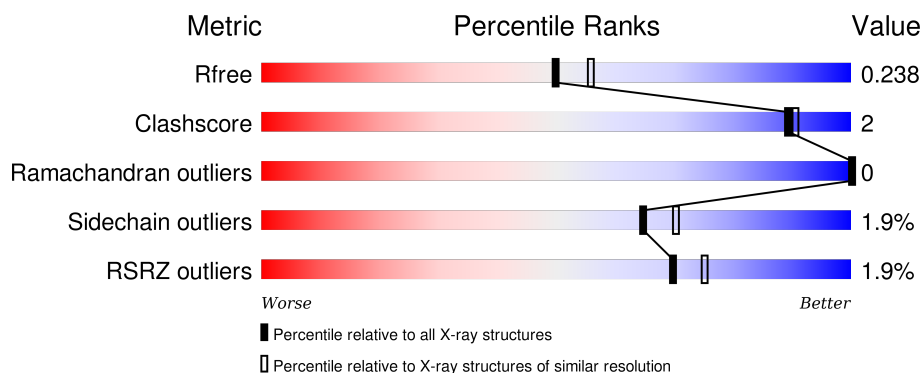
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	76	<div> <div>92%</div> <div>5% .</div> </div>
1	B	76	<div> <div>%</div> <div>97%</div> <div>..</div> </div>
1	C	76	<div> <div>%</div> <div>91%</div> <div>8% .</div> </div>
1	D	76	<div> <div>92%</div> <div>5% .</div> </div>
1	E	76	<div> <div>%</div> <div>91%</div> <div>7% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	76	
1	L	76	
1	M	76	
1	N	76	
1	O	76	

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
2	EFO	B	101	-	-	-	X
2	EFO	E	101	-	-	-	X
2	EFO	K	101	-	-	-	X
2	EFO	L	101	-	-	-	X
2	EFO	M	101	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6011 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 ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	3	0
			545	365	82	95	3			
1	B	75	Total	C	N	O	S	0	4	0
			554	372	83	96	3			
1	C	75	Total	C	N	O	S	0	3	0
			547	365	83	96	3			
1	D	74	Total	C	N	O	S	0	3	0
			545	365	82	95	3			
1	E	74	Total	C	N	O	S	0	3	0
			546	366	82	95	3			
1	K	75	Total	C	N	O	S	0	4	0
			551	369	83	96	3			
1	L	75	Total	C	N	O	S	0	3	0
			542	361	82	96	3			
1	M	75	Total	C	N	O	S	0	3	0
			543	361	83	96	3			
1	N	75	Total	C	N	O	S	0	3	0
			553	370	83	96	4			
1	O	75	Total	C	N	O	S	0	3	0
			550	368	83	96	3			

There are 10 discrepancies between the modelled and reference sequences:

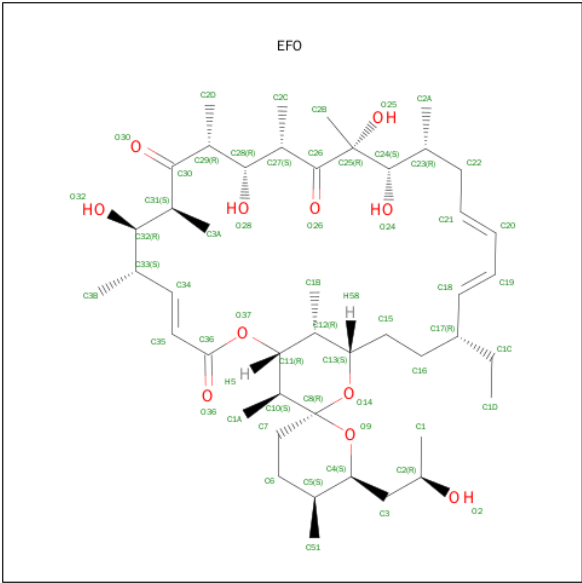
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	FME	-	initiating methionine	UNP P61829
B	1	FME	-	initiating methionine	UNP P61829
C	1	FME	-	initiating methionine	UNP P61829
D	1	FME	-	initiating methionine	UNP P61829
E	1	FME	-	initiating methionine	UNP P61829
K	1	FME	-	initiating methionine	UNP P61829
L	1	FME	-	initiating methionine	UNP P61829
M	1	FME	-	initiating methionine	UNP P61829
N	1	FME	-	initiating methionine	UNP P61829

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Chain	Residue	Modelled	Actual	Comment	Reference
O	1	FME	-	initiating methionine	UNP P61829

- Molecule 2 is Oligomycin A (three-letter code: EFO) (formula: C<sub>45</sub>H<sub>74</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 56 45 11	0	0
2	B	1	Total C O 56 45 11	0	0
2	E	1	Total C O 56 45 11	0	0
2	K	1	Total C O 56 45 11	0	0
2	L	1	Total C O 56 45 11	0	0
2	M	1	Total C O 56 45 11	0	0
2	O	1	Total C O 56 45 11	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	20	Total O 20 20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	20	Total 20	O 20	0	0
3	D	12	Total 12	O 12	0	0
3	E	12	Total 12	O 12	0	0
3	K	10	Total 10	O 10	0	0
3	L	13	Total 13	O 13	0	0
3	M	15	Total 15	O 15	0	0
3	N	13	Total 13	O 13	0	0
3	O	18	Total 18	O 18	0	0

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

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

- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain A:  92% 5% .

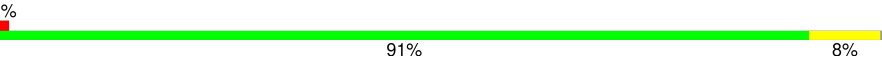


- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain B:  97% ..



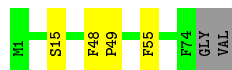
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain C:  91% 8% .




- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain D:  92% 5% .



- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain E:  91% 7% .

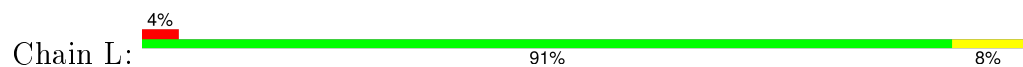


- Molecule 1: ATP synthase subunit 9, mitochondrial

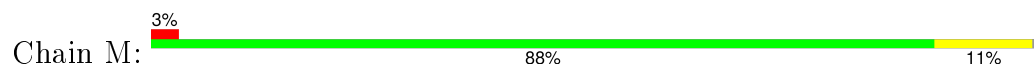
Chain K:  3% 95% ..



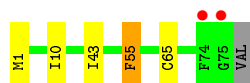
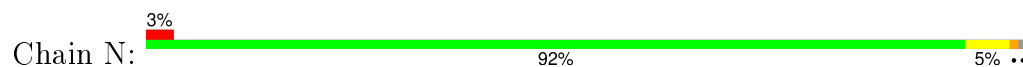
- Molecule 1: ATP synthase subunit 9, mitochondrial



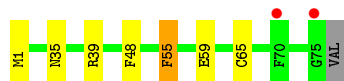
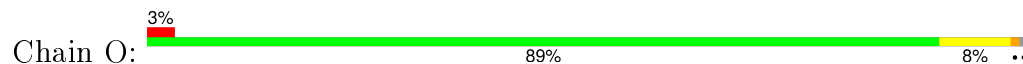
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.22Å 76.22Å 489.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 30.64 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.10) 99.8 (30.64-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.201 , 0.239 0.200 , 0.238	Depositor DCC
$R_{free}$ test set	2164 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 78.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	9 of 42907 reflections (0.021%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FME, EFO

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	0.46	0/561	0.57	0/760
1	B	0.47	0/573	0.50	0/776
1	C	0.46	0/562	0.52	0/761
1	D	0.46	0/561	0.53	0/760
1	E	0.47	0/561	0.52	0/760
1	K	0.45	0/570	0.51	0/772
1	L	0.44	0/558	0.51	0/757
1	M	0.45	0/558	0.55	0/756
1	N	0.45	0/566	0.51	0/766
1	O	0.46	0/565	0.52	0/765
All	All	0.46	0/5635	0.52	0/7633

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	A	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	FME	Mainchain
1	L	1	FME	Mainchain
1	M	1	FME	Mainchain
1	N	1	FME	Mainchain
1	O	1	FME	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	545	0	591	1	0
1	B	554	0	605	0	0
1	C	547	0	587	4	0
1	D	545	0	591	2	0
1	E	546	0	593	3	0
1	K	551	0	596	3	0
1	L	542	0	574	5	0
1	M	543	0	587	5	0
1	N	553	0	603	4	0
1	O	550	0	596	5	0
2	B	112	0	148	1	0
2	E	56	0	74	0	0
2	K	56	0	74	1	0
2	L	56	0	74	3	0
2	M	56	0	74	2	0
2	O	56	0	74	1	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	1	0
3	D	12	0	0	0	0
3	E	12	0	0	1	0
3	K	10	0	0	1	0
3	L	13	0	0	0	0
3	M	15	0	0	0	0
3	N	13	0	0	0	0
3	O	18	0	0	2	0
All	All	6011	0	6441	29	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 2.

All (29) 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:L:63:LEU:HA	2:L:101:EFO:H72	1.59	0.83
1:C:35[B]:ASN:HD21	1:C:39:ARG:HE	1.45	0.64
2:B:101:EFO:H57	1:C:59:GLU:HG2	1.85	0.57
1:O:39:ARG:HD2	3:O:202:HOH:O	2.07	0.55
1:C:35[B]:ASN:ND2	3:C:102:HOH:O	2.45	0.49
1:O:59:GLU:HG2	2:O:101:EFO:H57	1.95	0.47
1:M:40:ASN:O	1:M:43:ILE:HG22	2.14	0.47
1:A:35[B]:ASN:HD21	1:A:39:ARG:HE	1.63	0.46
1:L:10:ILE:HB	1:M:10:ILE:HD11	1.97	0.46
1:L:63:LEU:CA	2:L:101:EFO:H72	2.40	0.45
1:O:35[B]:ASN:ND2	3:O:202:HOH:O	2.50	0.45
1:E:40:ASN:O	1:E:43:ILE:HG22	2.18	0.43
1:N:55:PHE:C	1:N:55:PHE:CD1	2.93	0.43
1:K:63:LEU:HA	2:K:101:EFO:H72	2.01	0.43
1:K:15[C]:SER:OG	1:L:13:GLY:HA2	2.19	0.43
1:D:15[A]:SER:OG	1:E:13:GLY:HA2	2.19	0.42
1:D:48:PHE:HB3	1:D:49:PRO:HD3	2.01	0.42
1:M:7:ALA:HA	1:N:10:ILE:HD11	2.02	0.41
1:M:63:LEU:HD13	2:M:101:EFO:H68	2.02	0.41
1:M:59:GLU:HG2	2:M:101:EFO:H54	2.02	0.41
2:L:101:EFO:H7	2:L:101:EFO:H56	1.71	0.41
1:O:55:PHE:CD1	1:O:55:PHE:C	2.93	0.41
1:N:43:ILE:HD12	1:N:43:ILE:HA	1.88	0.41
1:K:35[A]:ASN:ND2	3:K:204:HOH:O	2.54	0.41
1:C:16:THR:O	1:C:19:LEU:HB2	2.21	0.40
1:E:35[B]:ASN:ND2	3:E:202:HOH:O	2.55	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	77/76 (101%)	77 (100%)	0	0	100	100
1	B	79/76 (104%)	79 (100%)	0	0	100	100
1	C	78/76 (103%)	77 (99%)	1 (1%)	0	100	100
1	D	77/76 (101%)	77 (100%)	0	0	100	100
1	E	77/76 (101%)	76 (99%)	1 (1%)	0	100	100
1	K	79/76 (104%)	79 (100%)	0	0	100	100
1	L	78/76 (103%)	78 (100%)	0	0	100	100
1	M	78/76 (103%)	78 (100%)	0	0	100	100
1	N	78/76 (103%)	78 (100%)	0	0	100	100
1	O	78/76 (103%)	78 (100%)	0	0	100	100
All	All	779/760 (102%)	777 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	58/55 (106%)	57 (98%)	1 (2%)	68	74
1	B	59/55 (107%)	58 (98%)	1 (2%)	68	74
1	C	57/55 (104%)	56 (98%)	1 (2%)	66	72
1	D	58/55 (106%)	57 (98%)	1 (2%)	68	74
1	E	58/55 (106%)	57 (98%)	1 (2%)	68	74
1	K	58/55 (106%)	58 (100%)	0	100	100
1	L	56/55 (102%)	55 (98%)	1 (2%)	66	72
1	M	57/55 (104%)	56 (98%)	1 (2%)	66	72
1	N	58/55 (106%)	57 (98%)	1 (2%)	68	74
1	O	58/55 (106%)	56 (97%)	2 (3%)	44	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	577/550 (105%)	567 (98%)	10 (2%)	65	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	B	55	PHE
1	C	55	PHE
1	D	55	PHE
1	E	55	PHE
1	L	55	PHE
1	M	55	PHE
1	N	55	PHE
1	O	48	PHE
1	O	55	PHE

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 ⓘ

10 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	FME	A	1	1	5,6,10	0.67	0	4,6,11	1.80	1 (25%)
1	FME	B	1	1	5,6,10	0.63	0	4,6,11	2.27	1 (25%)
1	FME	C	1	1	6,7,10	0.59	0	4,7,11	1.89	2 (50%)
1	FME	D	1	1	5,6,10	0.71	0	4,6,11	2.07	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	E	1	1	6,7,10	0.55	0	4,7,11	2.32	2 (50%)
1	FME	K	1	1	5,6,10	0.67	0	4,6,11	2.22	2 (50%)
1	FME	L	1	1	5,6,10	0.66	0	4,6,11	1.99	2 (50%)
1	FME	M	1	1	5,6,10	0.64	0	4,6,11	1.64	1 (25%)
1	FME	N	1	1	8,9,10	0.63	0	5,9,11	1.73	2 (40%)
1	FME	O	1	1	6,7,10	0.54	0	4,7,11	2.00	2 (50%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	0/2/5/11	0/0/0/0
1	FME	B	1	1	-	0/2/5/11	0/0/0/0
1	FME	C	1	1	-	0/4/7/11	0/0/0/0
1	FME	D	1	1	-	0/2/5/11	0/0/0/0
1	FME	E	1	1	-	0/4/7/11	0/0/0/0
1	FME	K	1	1	-	0/2/5/11	0/0/0/0
1	FME	L	1	1	-	0/2/5/11	0/0/0/0
1	FME	M	1	1	-	0/2/5/11	0/0/0/0
1	FME	N	1	1	-	0/6/9/11	0/0/0/0
1	FME	O	1	1	-	0/4/7/11	0/0/0/0

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	FME	O-C-CA	-3.98	117.71	124.97
1	K	1	FME	O-C-CA	-3.74	118.16	124.97
1	D	1	FME	O-C-CA	-3.69	118.25	124.97
1	E	1	FME	O1-CN-N	-3.51	119.44	124.80
1	L	1	FME	O-C-CA	-3.41	118.76	124.97
1	A	1	FME	O-C-CA	-3.13	119.28	124.97
1	N	1	FME	O1-CN-N	-2.99	120.22	124.80
1	O	1	FME	O-C-CA	-2.87	117.85	125.69
1	C	1	FME	O1-CN-N	-2.68	120.70	124.80
1	M	1	FME	O-C-CA	-2.63	120.18	124.97
1	E	1	FME	O-C-CA	-2.56	118.69	125.69
1	O	1	FME	O1-CN-N	-2.55	120.90	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O-C-CA	-2.32	119.36	125.69
1	K	1	FME	O1-CN-N	-2.31	121.26	124.80
1	C	1	FME	O-C-CA	-2.08	120.01	125.69
1	L	1	FME	O1-CN-N	-2.02	121.71	124.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
2	EFO	B	101	-	54,58,58	2.30	13 (24%)	55,85,85	1.39	4 (7%)
2	EFO	B	102	-	54,58,58	2.12	14 (25%)	55,85,85	1.09	4 (7%)
2	EFO	E	101	-	54,58,58	2.27	13 (24%)	55,85,85	1.21	7 (12%)
2	EFO	K	101	-	54,58,58	2.19	15 (27%)	55,85,85	1.27	7 (12%)
2	EFO	L	101	-	54,58,58	2.30	13 (24%)	55,85,85	1.52	7 (12%)
2	EFO	M	101	-	54,58,58	2.31	15 (27%)	55,85,85	1.32	6 (10%)
2	EFO	O	101	-	54,58,58	2.18	12 (22%)	55,85,85	1.11	5 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means



no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EFO	B	101	-	-	0/72/110/110	0/1/3/3
2	EFO	B	102	-	-	0/72/110/110	0/1/3/3
2	EFO	E	101	-	-	0/72/110/110	0/1/3/3
2	EFO	K	101	-	-	0/72/110/110	0/1/3/3
2	EFO	L	101	-	-	0/72/110/110	0/1/3/3
2	EFO	M	101	-	-	0/72/110/110	0/1/3/3
2	EFO	O	101	-	-	0/72/110/110	0/1/3/3

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	EFO	C25-C26	-8.30	1.42	1.54
2	E	101	EFO	C25-C26	-8.05	1.42	1.54
2	O	101	EFO	C25-C26	-7.97	1.42	1.54
2	L	101	EFO	C25-C26	-7.94	1.42	1.54
2	M	101	EFO	C25-C26	-7.58	1.43	1.54
2	B	101	EFO	C29-C30	-7.07	1.40	1.52
2	B	102	EFO	C25-C26	-7.03	1.44	1.54
2	L	101	EFO	C31-C30	-6.92	1.41	1.52
2	K	101	EFO	C25-C26	-6.63	1.44	1.54
2	M	101	EFO	C29-C30	-6.40	1.41	1.52
2	O	101	EFO	C31-C30	-6.33	1.42	1.52
2	K	101	EFO	C31-C30	-6.23	1.42	1.52
2	E	101	EFO	C29-C30	-6.12	1.42	1.52
2	B	102	EFO	C31-C30	-6.09	1.42	1.52
2	M	101	EFO	C31-C30	-6.09	1.42	1.52
2	L	101	EFO	C29-C30	-6.08	1.42	1.52
2	E	101	EFO	C31-C30	-6.04	1.42	1.52
2	B	101	EFO	C31-C30	-5.99	1.42	1.52
2	K	101	EFO	C29-C30	-5.72	1.43	1.52
2	O	101	EFO	C29-C30	-5.43	1.43	1.52
2	B	102	EFO	C29-C30	-4.90	1.44	1.52
2	M	101	EFO	C33-C34	-4.63	1.39	1.51
2	B	101	EFO	C33-C34	-4.53	1.39	1.51
2	E	101	EFO	C33-C34	-4.50	1.39	1.51
2	L	101	EFO	C33-C34	-4.45	1.39	1.51
2	L	101	EFO	C17-C18	-4.40	1.40	1.50
2	K	101	EFO	C17-C18	-4.32	1.40	1.50
2	B	101	EFO	C17-C18	-4.26	1.40	1.50
2	O	101	EFO	C33-C34	-4.22	1.40	1.51
2	M	101	EFO	C17-C18	-4.16	1.40	1.50
2	M	101	EFO	C22-C21	-3.96	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	101	EFO	C33-C34	-3.88	1.41	1.51
2	B	102	EFO	C17-C18	-3.87	1.41	1.50
2	M	101	EFO	C35-C36	-3.85	1.39	1.48
2	B	102	EFO	C33-C34	-3.81	1.41	1.51
2	L	101	EFO	C22-C21	-3.80	1.39	1.50
2	E	101	EFO	C17-C18	-3.78	1.41	1.50
2	K	101	EFO	C22-C21	-3.75	1.39	1.50
2	E	101	EFO	C35-C36	-3.73	1.39	1.48
2	L	101	EFO	C35-C36	-3.66	1.39	1.48
2	O	101	EFO	C35-C36	-3.51	1.40	1.48
2	B	101	EFO	C35-C36	-3.50	1.40	1.48
2	B	101	EFO	C22-C21	-3.42	1.40	1.50
2	K	101	EFO	C35-C36	-3.28	1.40	1.48
2	E	101	EFO	C22-C21	-3.25	1.41	1.50
2	B	102	EFO	C35-C36	-3.15	1.41	1.48
2	O	101	EFO	C17-C18	-3.08	1.43	1.50
2	B	102	EFO	C22-C21	-3.03	1.41	1.50
2	M	101	EFO	C27-C26	-2.92	1.42	1.53
2	O	101	EFO	C22-C21	-2.74	1.42	1.50
2	B	101	EFO	C27-C26	-2.72	1.42	1.53
2	L	101	EFO	C27-C26	-2.70	1.43	1.53
2	O	101	EFO	C27-C26	-2.67	1.43	1.53
2	E	101	EFO	C27-C26	-2.63	1.43	1.53
2	K	101	EFO	C27-C26	-2.62	1.43	1.53
2	B	102	EFO	C27-C26	-2.08	1.45	1.53
2	M	101	EFO	C19-C20	-2.03	1.38	1.44
2	M	101	EFO	C12-C11	2.00	1.57	1.53
2	B	101	EFO	O9-C8	2.03	1.47	1.42
2	K	101	EFO	O14-C8	2.04	1.47	1.42
2	B	101	EFO	C7-C8	2.05	1.55	1.52
2	L	101	EFO	O14-C8	2.05	1.47	1.42
2	K	101	EFO	C20-C21	2.08	1.39	1.32
2	O	101	EFO	O14-C8	2.08	1.47	1.42
2	E	101	EFO	C7-C8	2.14	1.55	1.52
2	M	101	EFO	C20-C21	2.15	1.39	1.32
2	B	102	EFO	C20-C21	2.17	1.39	1.32
2	L	101	EFO	C20-C21	2.17	1.39	1.32
2	B	102	EFO	C22-C23	2.18	1.57	1.54
2	E	101	EFO	O14-C8	2.18	1.47	1.42
2	B	101	EFO	O14-C8	2.22	1.47	1.42
2	B	101	EFO	C20-C21	2.22	1.39	1.32
2	M	101	EFO	C31-C32	2.24	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	101	EFO	O9-C8	2.24	1.47	1.42
2	K	101	EFO	O9-C4	2.27	1.49	1.44
2	O	101	EFO	C20-C21	2.31	1.39	1.32
2	M	101	EFO	O14-C8	2.34	1.47	1.42
2	K	101	EFO	C7-C8	2.34	1.56	1.52
2	B	102	EFO	C31-C32	2.36	1.58	1.54
2	K	101	EFO	C31-C32	2.44	1.59	1.54
2	O	101	EFO	C7-C8	2.44	1.56	1.52
2	E	101	EFO	C31-C32	2.44	1.59	1.54
2	B	102	EFO	C29-C28	2.44	1.59	1.54
2	B	102	EFO	C7-C8	2.46	1.56	1.52
2	E	101	EFO	C20-C21	2.48	1.40	1.32
2	L	101	EFO	C7-C8	2.57	1.56	1.52
2	M	101	EFO	C7-C8	2.61	1.56	1.52
2	M	101	EFO	C35-C34	2.69	1.39	1.32
2	K	101	EFO	O9-C8	2.74	1.48	1.42
2	B	101	EFO	C35-C34	2.81	1.39	1.32
2	E	101	EFO	C35-C34	2.83	1.39	1.32
2	L	101	EFO	C35-C34	2.84	1.39	1.32
2	O	101	EFO	C35-C34	2.90	1.39	1.32
2	K	101	EFO	C35-C34	3.11	1.40	1.32
2	B	102	EFO	C35-C34	3.23	1.40	1.32

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	101	EFO	C15-C16-C17	-3.81	107.57	113.75
2	K	101	EFO	C23-C22-C21	-3.43	108.47	113.71
2	K	101	EFO	C2C-C27-C28	-3.23	106.59	112.46
2	L	101	EFO	C23-C22-C21	-3.13	108.92	113.71
2	B	102	EFO	C23-C22-C21	-2.86	109.34	113.71
2	M	101	EFO	C11-O37-C36	-2.84	112.94	117.16
2	O	101	EFO	C16-C15-C13	-2.67	108.15	113.34
2	O	101	EFO	C2C-C27-C28	-2.59	107.75	112.46
2	E	101	EFO	C16-C15-C13	-2.55	108.38	113.34
2	K	101	EFO	C15-C16-C17	-2.52	109.66	113.75
2	B	102	EFO	C2C-C27-C28	-2.51	107.89	112.46
2	O	101	EFO	C23-C22-C21	-2.48	109.92	113.71
2	L	101	EFO	C2C-C27-C28	-2.41	108.08	112.46
2	E	101	EFO	C2C-C27-C28	-2.30	108.28	112.46
2	E	101	EFO	C34-C35-C36	-2.26	117.18	122.71
2	L	101	EFO	C11-O37-C36	-2.25	113.82	117.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	101	EFO	C23-C22-C21	-2.14	110.43	113.71
2	K	101	EFO	C34-C35-C36	-2.04	117.72	122.71
2	B	101	EFO	C2C-C27-C28	-2.02	108.80	112.46
2	E	101	EFO	O37-C36-C35	2.01	116.36	111.39
2	B	102	EFO	O37-C36-C35	2.03	116.41	111.39
2	M	101	EFO	C32-C31-C30	2.15	113.48	109.89
2	E	101	EFO	C31-C30-C29	2.15	122.12	118.11
2	K	101	EFO	O37-C36-C35	2.16	116.72	111.39
2	L	101	EFO	O37-C36-C35	2.44	117.42	111.39
2	B	101	EFO	O37-C36-C35	2.50	117.56	111.39
2	M	101	EFO	O37-C36-C35	2.67	117.98	111.39
2	O	101	EFO	O14-C13-C15	2.69	109.11	106.02
2	O	101	EFO	O9-C4-C3	2.86	109.84	105.80
2	E	101	EFO	O14-C13-C15	3.30	109.82	106.02
2	K	101	EFO	O14-C13-C15	3.43	109.97	106.02
2	B	102	EFO	O14-C13-C15	3.63	110.20	106.02
2	K	101	EFO	O9-C4-C3	4.14	111.65	105.80
2	M	101	EFO	O9-C4-C3	4.26	111.84	105.80
2	M	101	EFO	O14-C13-C15	4.36	111.04	106.02
2	E	101	EFO	O9-C4-C3	4.43	112.08	105.80
2	L	101	EFO	O14-C13-C15	4.81	111.56	106.02
2	B	101	EFO	O9-C4-C3	5.23	113.20	105.80
2	B	101	EFO	O14-C13-C15	5.35	112.18	106.02
2	L	101	EFO	O9-C4-C3	5.39	113.44	105.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	101	EFO	1	0
2	K	101	EFO	1	0
2	L	101	EFO	3	0
2	M	101	EFO	2	0
2	O	101	EFO	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	73/76 (96%)	-0.26	0 <span>100</span> <span>100</span>	15, 21, 39, 50	0
1	B	74/76 (97%)	-0.33	1 (1%) <span>78</span> <span>82</span>	15, 21, 39, 46	0
1	C	74/76 (97%)	-0.31	1 (1%) <span>78</span> <span>82</span>	15, 22, 41, 52	0
1	D	73/76 (96%)	-0.53	0 <span>100</span> <span>100</span>	14, 22, 38, 44	0
1	E	73/76 (96%)	-0.32	1 (1%) <span>78</span> <span>82</span>	15, 22, 40, 47	0
1	K	74/76 (97%)	-0.20	2 (2%) <span>58</span> <span>65</span>	16, 25, 51, 57	0
1	L	74/76 (97%)	-0.17	3 (4%) <span>41</span> <span>50</span>	16, 28, 53, 58	0
1	M	74/76 (97%)	-0.10	2 (2%) <span>58</span> <span>65</span>	16, 28, 53, 69	0
1	N	74/76 (97%)	-0.24	2 (2%) <span>58</span> <span>65</span>	16, 25, 49, 58	0
1	O	74/76 (97%)	-0.11	2 (2%) <span>58</span> <span>65</span>	16, 25, 50, 56	0
All	All	737/760 (96%)	-0.26	14 (1%) <span>70</span> <span>75</span>	14, 23, 48, 69	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	75	GLY	3.2
1	M	5	LEU	3.1
1	B	75	GLY	2.9
1	E	70	PHE	2.8
1	O	75	GLY	2.8
1	L	75	GLY	2.7
1	C	75	GLY	2.6
1	K	75	GLY	2.5
1	O	70	PHE	2.4
1	M	70	PHE	2.4
1	L	74	PHE	2.3
1	L	70	PHE	2.2
1	N	74	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	70	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	FME	A	1	7/11	0.81	0.19	-	47,49,52,56	0
1	FME	L	1	7/11	0.63	0.32	-	60,63,66,70	0
1	FME	N	1	10/11	0.67	0.31	-	56,64,72,73	0
1	FME	B	1	7/11	0.32	0.28	-	49,50,54,58	0
1	FME	M	1	7/11	0.75	0.20	-	55,57,60,65	0
1	FME	D	1	7/11	0.42	0.32	-	45,47,51,53	0
1	FME	K	1	7/11	0.75	0.33	-	62,65,68,70	0
1	FME	E	1	8/11	0.83	0.28	-	47,49,54,58	0
1	FME	O	1	8/11	0.84	0.28	-	57,59,64,66	0
1	FME	C	1	8/11	0.81	0.19	-	50,53,57,59	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EFO	L	101	56/56	0.64	0.42	10.80	41,55,61,63	0
2	EFO	B	101	56/56	0.65	0.31	7.92	42,49,56,60	0
2	EFO	M	101	56/56	0.76	0.23	3.43	33,44,50,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EFO	K	101	56/56	0.78	0.19	2.55	31,34,38,39	0
2	EFO	E	101	56/56	0.87	0.16	2.24	28,32,36,37	0
2	EFO	B	102	56/56	0.88	0.13	1.55	21,25,34,36	0
2	EFO	O	101	56/56	0.86	0.14	1.33	21,28,32,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.