



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:32 PM GMT

PDB ID : 3RFR  
Title : Crystal Structure of particulate methane monooxygenase (pMMO) from  
Methylocystis sp. strain M  
Authors : Smith, S.M.; Rosenzweig, A.C.  
Deposited on : 2011-04-06  
Resolution : 2.68 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

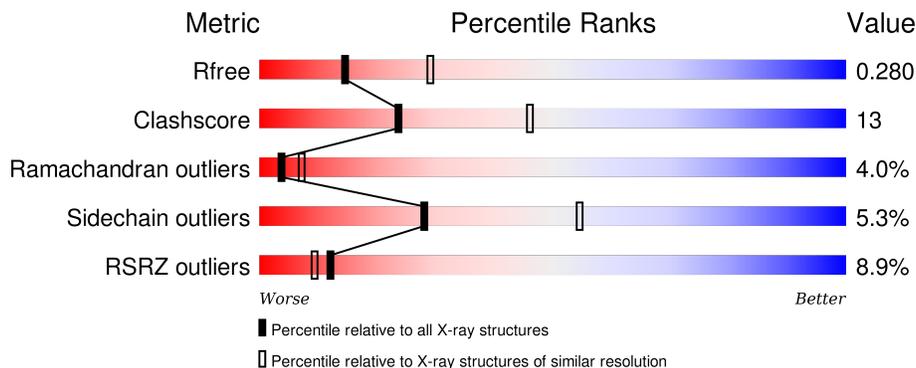
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	419	 9% 68% 19% •• 8%
1	E	419	 9% 68% 19% •• 8%
1	I	419	 12% 56% 31% •• 8%
2	D	19	 11% 74% 26%
2	H	19	 26% 68% 16% 16%

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Mol	Chain	Length	Quality of chain
3	B	252	<p>6% 70% 22% . . .</p>
3	F	252	<p>7% 69% 22% . . .</p>
3	J	252	<p>4% 69% 21% 5% . .</p>
4	C	256	<p>8% 60% 19% . . 18%</p>
4	G	256	<p>5% 60% 20% . . 18%</p>
4	K	256	<p>7% 63% 17% . . 18%</p>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 20224 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 PmoB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3012	1937	521	551	3	0	0	0
1	E	386	3012	1937	521	551	3	0	0	0
1	I	386	3012	1937	521	551	3	0	0	0

- Molecule 2 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	19	94	57	19	18	0	0	0
2	H	16	79	48	16	15	0	0	0

- Molecule 3 is a protein called PmoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	J	242	1964	1326	312	313	13	0	0	0
3	B	242	1964	1326	312	313	13	0	0	0
3	F	242	1964	1326	312	313	13	0	0	0

- Molecule 4 is a protein called PmoC.

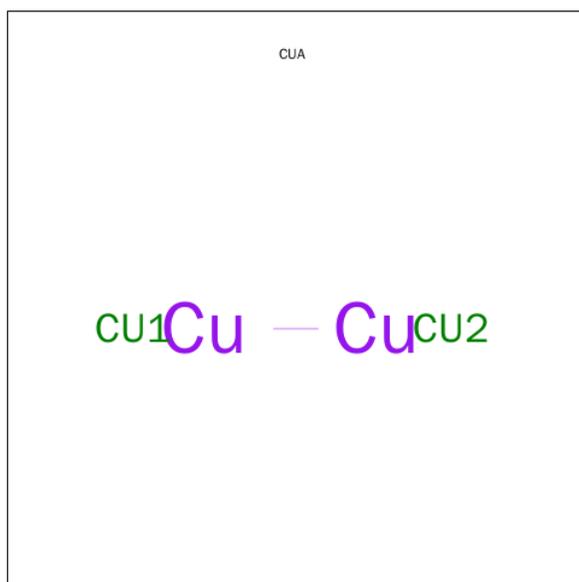
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	210	1695	1137	271	280	7	0	0	0
4	G	211	1706	1146	272	281	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	K	211	1706	1146	272	281	7	0	0	0

- Molecule 5 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			2	2		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total	Zn	0	0
			2	2		
6	K	2	Total	Zn	0	0
			2	2		
6	E	1	Total	Zn	0	0
			1	1		
6	I	1	Total	Zn	0	0
			1	1		
6	C	2	Total	Zn	0	0
			2	2		
6	A	1	Total	Zn	0	0
			1	1		

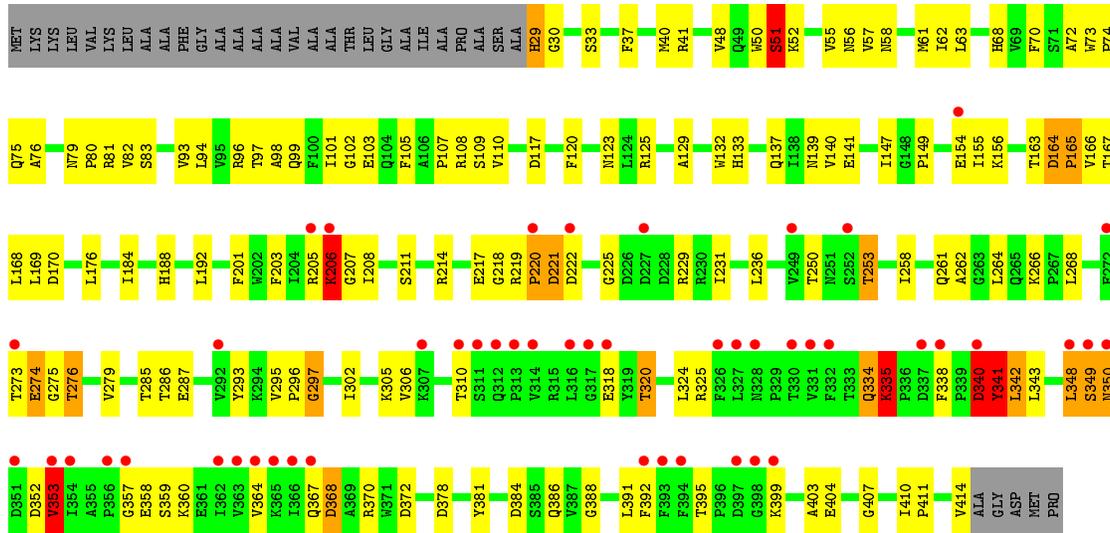
- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total Cu 1 1	0	0
7	E	1	Total Cu 1 1	0	0

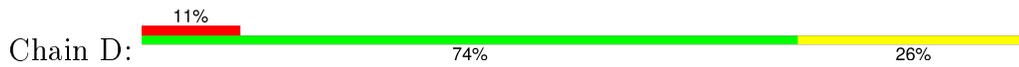
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O 1 1	0	0
8	G	1	Total O 1 1	0	0
8	K	1	Total O 1 1	0	0





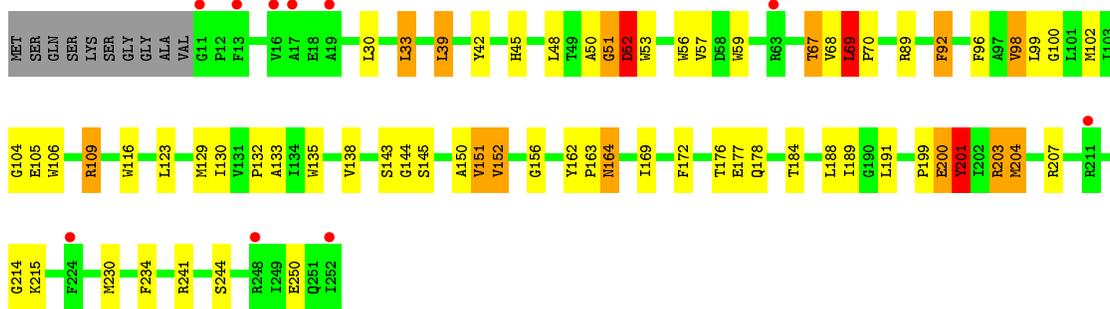
• Molecule 2: peptide



• Molecule 2: peptide

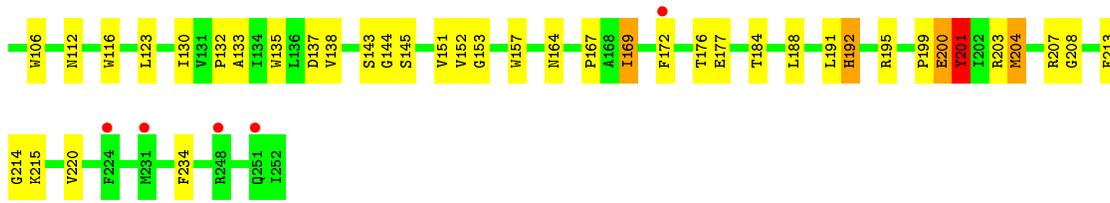


• Molecule 3: PmoA

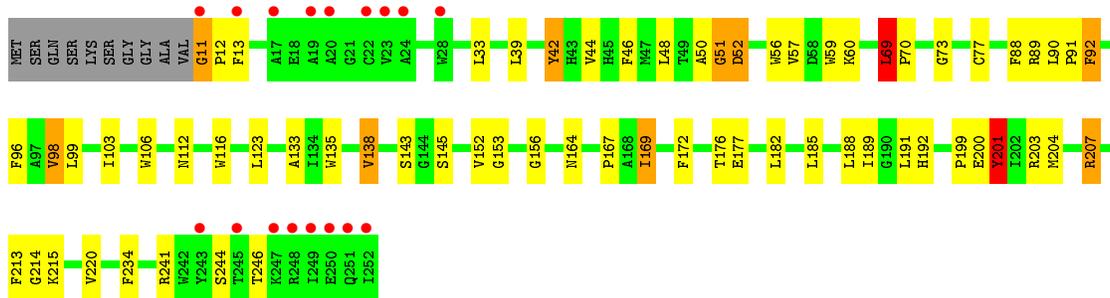


• Molecule 3: PmoA

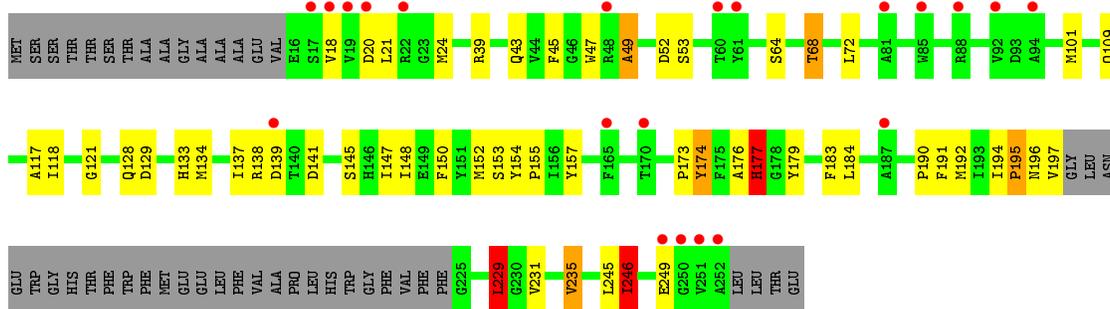




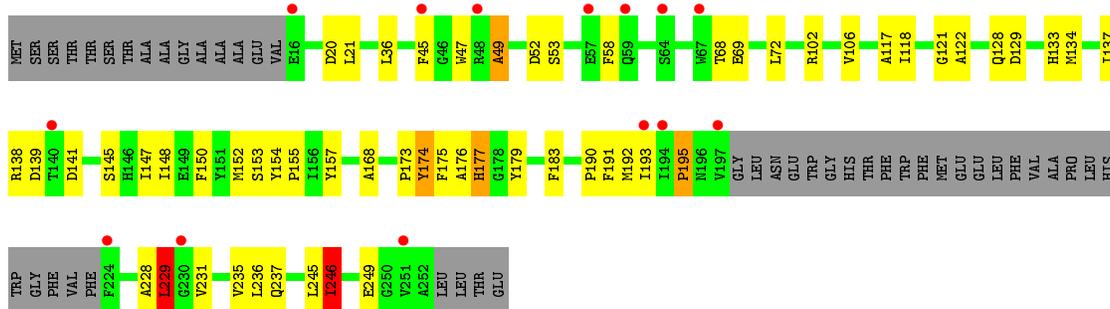
• Molecule 3: PmoA



• Molecule 4: PmoC

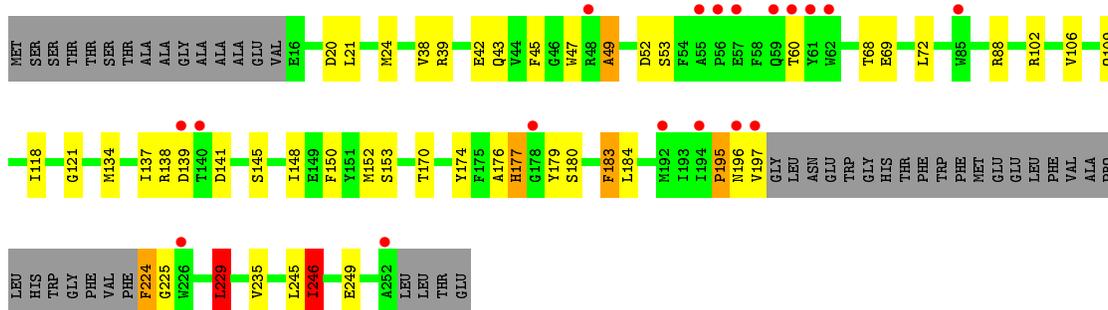


• Molecule 4: PmoC



• Molecule 4: PmoC





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.72Å 178.31Å 183.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 2.68 45.79 – 2.68	Depositor EDS
% Data completeness (in resolution range)	88.9 (45.79-2.68) 88.9 (45.79-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.249 , 0.281 0.250 , 0.280	Depositor DCC
$R_{free}$ test set	4440 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.6	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 88166 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	20224	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CUA, CU

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	0.66	0/3087	0.81	4/4205 (0.1%)
1	E	0.69	0/3087	0.81	5/4205 (0.1%)
1	I	1.04	1/3087 (0.0%)	0.94	4/4205 (0.1%)
2	D	1.00	0/93	1.02	0/129
2	H	0.84	0/78	0.67	0/108
3	B	0.79	0/2041	0.81	2/2795 (0.1%)
3	F	0.86	0/2041	0.86	2/2795 (0.1%)
3	J	0.92	0/2041	0.89	3/2795 (0.1%)
4	C	0.70	0/1749	0.70	1/2386 (0.0%)
4	G	0.66	0/1761	0.69	1/2402 (0.0%)
4	K	0.72	0/1761	0.72	2/2402 (0.1%)
All	All	0.80	1/20826 (0.0%)	0.82	24/28427 (0.1%)

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	4
1	E	0	3
1	I	0	4
3	B	0	3
3	F	0	3
3	J	0	2
4	G	0	1
4	K	0	1
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	154	GLU	CG-CD	5.42	1.60	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	69	LEU	CA-CB-CG	-7.86	97.23	115.30
3	F	69	LEU	CA-CB-CG	-7.58	97.87	115.30
3	J	69	LEU	CA-CB-CG	-7.37	98.34	115.30
4	G	229	LEU	CA-CB-CG	6.79	130.93	115.30
4	C	229	LEU	CA-CB-CG	6.76	130.85	115.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	LYS	Peptide
1	A	308	ASN	Peptide
1	A	335	LYS	Peptide
1	A	340	ASP	Peptide
3	J	50	ALA	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	3012	0	3009	94	0
1	E	3012	0	3009	95	0
1	I	3012	0	3009	136	0
2	D	94	0	97	2	0
2	H	79	0	79	2	0
3	B	1964	0	1924	55	0
3	F	1964	0	1924	62	0
3	J	1964	0	1924	55	0
4	C	1695	0	1692	36	0
4	G	1706	0	1701	36	0
4	K	1706	0	1701	36	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2	0	0	0	0
6	E	1	0	0	0	0
6	G	2	0	0	0	0
6	I	1	0	0	0	0
6	K	2	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
8	C	1	0	0	0	0
8	G	1	0	0	0	0
8	K	1	0	0	0	0
All	All	20224	0	20069	533	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 13.

The worst 5 of 533 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)
3:J:116:TRP:O	4:K:47:TRP:HH2	1.31	1.13
1:I:275:GLY:HA3	1:I:276:THR:HG22	1.29	1.11
3:F:11:GLY:HA3	3:F:13:PHE:H	1.02	1.10
1:A:340:ASP:HB3	1:A:341:TYR:HB3	1.33	1.09
3:B:51:GLY:HA3	3:B:52:ASP:HB2	1.28	1.08

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	384/419 (92%)	338 (88%)	27 (7%)	19 (5%)	<b>3</b> <b>4</b>
1	E	384/419 (92%)	340 (88%)	26 (7%)	18 (5%)	<b>3</b> <b>5</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	384/419 (92%)	330 (86%)	31 (8%)	23 (6%)	2	2
2	D	17/19 (90%)	13 (76%)	2 (12%)	2 (12%)	0	0
2	H	14/19 (74%)	12 (86%)	2 (14%)	0	100	100
3	B	240/252 (95%)	218 (91%)	16 (7%)	6 (2%)	7	16
3	F	240/252 (95%)	215 (90%)	22 (9%)	3 (1%)	15	35
3	J	240/252 (95%)	214 (89%)	19 (8%)	7 (3%)	6	13
4	C	206/256 (80%)	188 (91%)	10 (5%)	8 (4%)	4	7
4	G	207/256 (81%)	181 (87%)	18 (9%)	8 (4%)	4	7
4	K	207/256 (81%)	184 (89%)	16 (8%)	7 (3%)	5	10
All	All	2523/2819 (90%)	2233 (88%)	189 (8%)	101 (4%)	4	7

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	164	ASP
1	A	220	PRO
1	A	221	ASP
1	A	274	GLU

### 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	318/335 (95%)	305 (96%)	13 (4%)	37	66
1	E	318/335 (95%)	304 (96%)	14 (4%)	35	63
1	I	318/335 (95%)	304 (96%)	14 (4%)	35	63
3	B	201/208 (97%)	187 (93%)	14 (7%)	19	40
3	F	201/208 (97%)	186 (92%)	15 (8%)	17	36
3	J	201/208 (97%)	187 (93%)	14 (7%)	19	40
4	C	173/209 (83%)	163 (94%)	10 (6%)	25	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	174/209 (83%)	166 (95%)	8 (5%)	33	61
4	K	174/209 (83%)	165 (95%)	9 (5%)	29	55
All	All	2078/2256 (92%)	1967 (95%)	111 (5%)	28	54

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	152	VAL
4	C	183	PHE
1	I	253	THR
3	F	164	ASN
4	C	68	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	G	109	GLN
4	K	128	GLN
1	I	188	HIS
4	G	128	GLN
4	G	177	HIS

### 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 carbohydrates in this entry.

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

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 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	$\# Z  > 2$
5	CUA	A	420	1	0,1,1	0.00	-	0,0,0	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
5	CUA	A	420	1	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	386/419 (92%)	0.51	38 (9%) 10 7	50, 69, 98, 114	0
1	E	386/419 (92%)	0.52	38 (9%) 10 7	48, 68, 101, 123	0
1	I	386/419 (92%)	0.45	49 (12%) 5 4	34, 50, 74, 90	0
2	D	19/19 (100%)	0.39	2 (10%) 8 6	78, 80, 83, 83	0
2	H	16/19 (84%)	1.52	5 (31%) 1 0	97, 99, 104, 104	0
3	B	242/252 (96%)	0.29	14 (5%) 26 24	43, 58, 90, 109	0
3	F	242/252 (96%)	0.44	17 (7%) 19 17	42, 57, 93, 117	0
3	J	242/252 (96%)	0.11	10 (4%) 41 39	40, 55, 89, 109	0
4	C	210/256 (82%)	0.56	21 (10%) 9 6	53, 69, 101, 114	0
4	G	211/256 (82%)	0.46	14 (6%) 22 19	53, 78, 112, 125	0
4	K	211/256 (82%)	0.50	18 (8%) 13 10	54, 72, 106, 119	0
All	All	2551/2819 (90%)	0.44	226 (8%) 12 9	34, 63, 100, 125	0

The worst 5 of 226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	394	PHE	8.4
4	K	56	PRO	7.4
1	I	349	SER	7.4
1	I	365	LYS	7.0
3	B	11	GLY	6.9

### 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 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
6	ZN	I	421	1/1	0.97	0.28	0.42	70,70,70,70	0
5	CUA	A	420	2/2	0.96	0.11	-2.27	72,72,72,93	0
7	CU	E	420	1/1	0.96	0.04	-	63,63,63,63	0
7	CU	I	420	1/1	0.95	0.08	-	76,76,76,76	0
6	ZN	K	258	1/1	0.80	0.20	-	141,141,141,141	0
6	ZN	K	257	1/1	0.99	0.10	-	70,70,70,70	0
6	ZN	C	257	1/1	0.99	0.11	-	57,57,57,57	0
6	ZN	G	258	1/1	0.82	0.11	-	129,129,129,129	0
6	ZN	G	257	1/1	0.98	0.14	-	64,64,64,64	0
6	ZN	C	258	1/1	0.97	0.03	-	87,87,87,87	0
6	ZN	E	421	1/1	0.98	0.08	-	90,90,90,90	0
6	ZN	A	421	1/1	0.93	0.08	-	88,88,88,88	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.