



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:37 PM GMT

PDB ID : 3RGB  
Title : Crystal structure of particulate methane monooxygenase from *Methylococcus capsulatus* (Bath)  
Authors : Smith, S.M.; Rosenzweig, A.C.  
Deposited on : 2011-04-08  
Resolution : 2.80 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

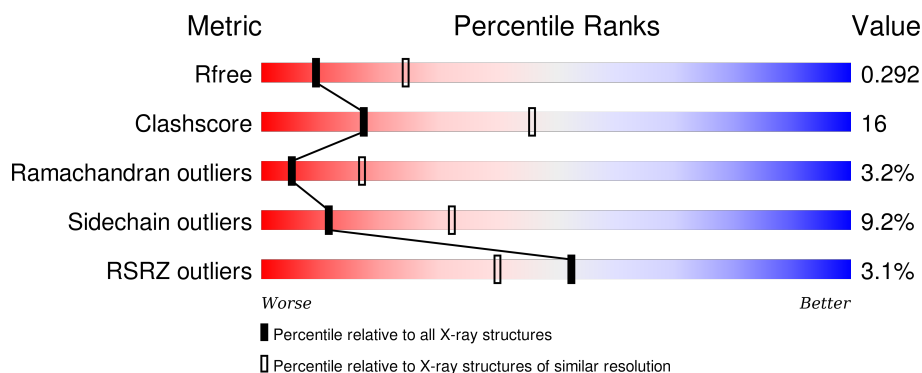
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	414	<div> <div> <div></div> <div>56%</div> <div>32%</div> <div>• • 8%</div> </div> </div>
1	E	414	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>26%</div> <div>5%</div> <div>8%</div> </div> </div>
1	I	414	<div> <div> <div></div> <div>63%</div> <div>25%</div> <div>• 8%</div> </div> </div>
2	B	247	<div> <div> <div></div> <div>54%</div> <div>28%</div> <div>6%</div> <div>12%</div> </div> </div>
2	F	247	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>30%</div> <div>5%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	J	247	<div><div></div><div>2%</div><div>55%</div><div>28%</div><div>• •</div><div>12%</div></div>
3	C	289	<div><div></div><div>3%</div><div>43%</div><div>24%</div><div>6%</div><div>26%</div></div>
3	G	289	<div><div></div><div>5%</div><div>48%</div><div>20%</div><div>• •</div><div>26%</div></div>
3	K	289	<div><div></div><div>7%</div><div>46%</div><div>21%</div><div>6%</div><div>26%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19737 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 Methane monooxygenase subunit B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3017	1938	513	551	15			
1	E	382	Total	C	N	O	S	0	0	0
			3017	1938	513	551	15			
1	I	382	Total	C	N	O	S	0	0	0
			3017	1938	513	551	15			

- Molecule 2 is a protein called Methane monooxygenase subunit A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1796	1216	284	286	10			
2	J	218	Total	C	N	O	S	0	0	0
			1796	1216	284	286	10			
2	F	218	Total	C	N	O	S	0	0	0
			1796	1216	284	286	10			

- Molecule 3 is a protein called Methane monooxygenase subunit C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1759	1187	268	300	4			
3	K	213	Total	C	N	O	S	0	0	0
			1759	1187	268	300	4			
3	G	213	Total	C	N	O	S	0	0	0
			1759	1187	268	300	4			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Cu	0	0
			1	1		

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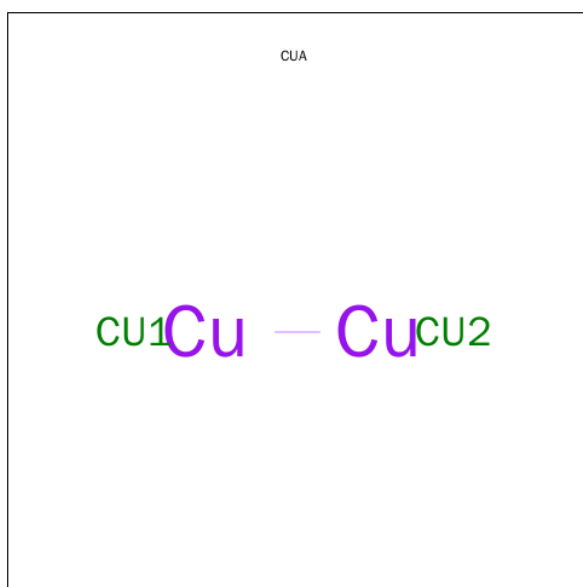
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		
4	E	1	Total	Cu	0	0
			1	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Zn	0	0
			1	1		
5	J	1	Total	Zn	0	0
			1	1		
5	K	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	I	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		

- Molecule 6 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cu 2 2	0	0
6	E	1	Total Cu 2 2	0	0
6	I	1	Total Cu 2 2	0	0

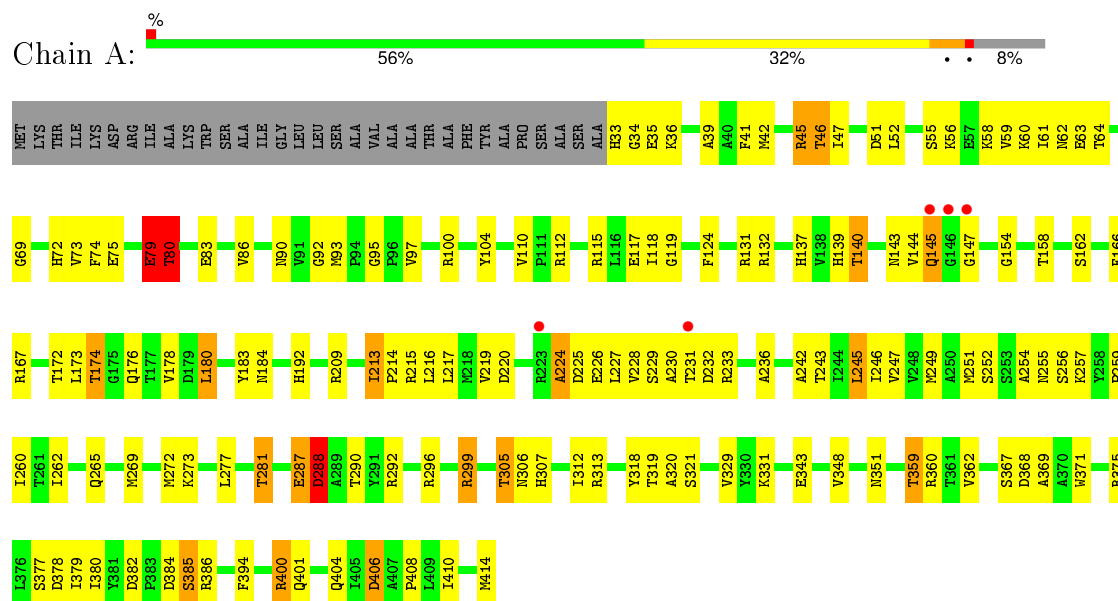
- Molecule 7 is water.

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

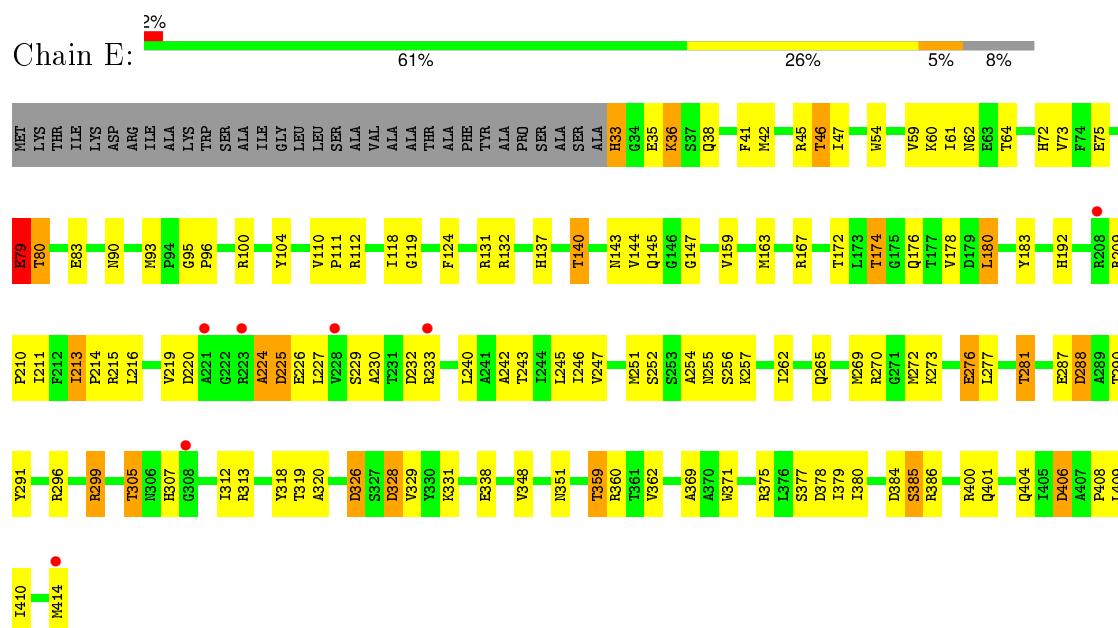
### 3 Residue-property plots

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: Methane monooxygenase subunit B2



#### • Molecule 1: Methane monooxygenase subunit B2



Chain I:

63% 25% 8%

Label	Value
T830	12.16
N90	12.16
N93	12.16
P94	12.16
G95	12.16
Y104	12.16
V110	12.16
P111	12.16
R112	12.16
I118	12.16
G119	12.16
F124	12.16
H137	12.16
T140	12.16
N143	12.16
V144	12.16
Q145	12.16
G146	12.16
G147	12.16
V159	12.16
S162	12.16
R167	12.16
T172	12.16
L173	12.16
T174	12.16
G175	12.16
Q176	12.16
T177	12.16
V178	12.16
L180	12.16
Y183	12.16
N184	12.16
T188	12.16
H192	12.16
R208	12.16
R209	12.16
T210	12.16
I211	12.16
F212	12.16
I213	12.16
P214	12.16
P215	12.16
P216	12.16
P217	12.16
P218	12.16
P219	12.16
P220	12.16
P221	12.16
P222	12.16
P223	12.16
P224	12.16
P225	12.16
P226	12.16
P227	12.16
P228	12.16
P229	12.16
P230	12.16
P231	12.16
P232	12.16
P233	12.16
P234	12.16
P235	12.16
P236	12.16
P237	12.16
P238	12.16
P239	12.16
P240	12.16
P241	12.16
P242	12.16
P243	12.16
P244	12.16
P245	12.16
P246	12.16
P247	12.16
P248	12.16
P249	12.16
P250	12.16
P251	12.16
P252	12.16
P253	12.16
P254	12.16
P255	12.16
P256	12.16
P257	12.16
P258	12.16
P259	12.16
P260	12.16
P261	12.16
P262	12.16
P263	12.16
P264	12.16
P265	12.16
P266	12.16
P267	12.16
P268	12.16
P269	12.16
P270	12.16
P271	12.16
P272	12.16
P273	12.16
P274	12.16
P275	12.16
P276	12.16
P277	12.16
P278	12.16
P279	12.16
P280	12.16
P281	12.16
P282	12.16
P283	12.16
P284	12.16
P285	12.16
P286	12.16
P287	12.16
P288	12.16
P289	12.16
P290	12.16
P291	12.16
P292	12.16
P293	12.16
P294	12.16
P295	12.16
P296	12.16
P297	12.16
P298	12.16
P299	12.16
P300	12.16
P301	12.16
P302	12.16
P303	12.16
P304	12.16
P305	12.16
P306	12.16
P307	12.16
P308	12.16
P309	12.16
P310	12.16
P311	12.16
P312	12.16
P313	12.16
P314	12.16
P315	12.16
P316	12.16
P317	12.16
P318	12.16
P319	12.16
P320	12.16
P321	12.16
P322	12.16
P323	12.16
P324	12.16
P325	12.16
P326	12.16
P327	12.16
P328	12.16
P329	12.16
P330	12.16
P331	12.16
P332	12.16
P333	12.16
P334	12.16
P335	12.16
P336	12.16
P337	12.16
P338	12.16
P339	12.16
P340	12.16
P341	12.16
P342	12.16
P343	12.16
P344	12.16
P345	12.16
P346	12.16
P347	12.16
P348	12.16
P349	12.16
P350	12.16
P351	12.16
P352	12.16
P35	

[illegible]

Chain J:

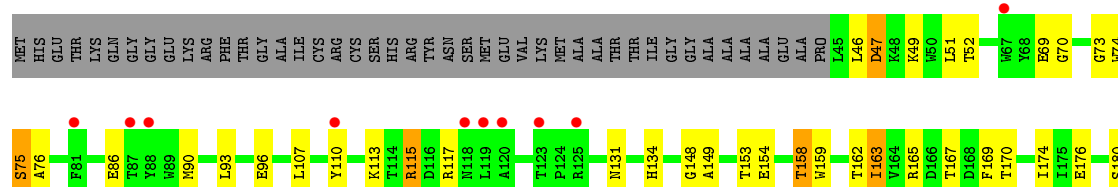
Sequence logo for Chain J. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 190. A color scale at the top indicates conservation levels: 2% (red), 55% (yellow), 28% (orange), and 12% (grey).

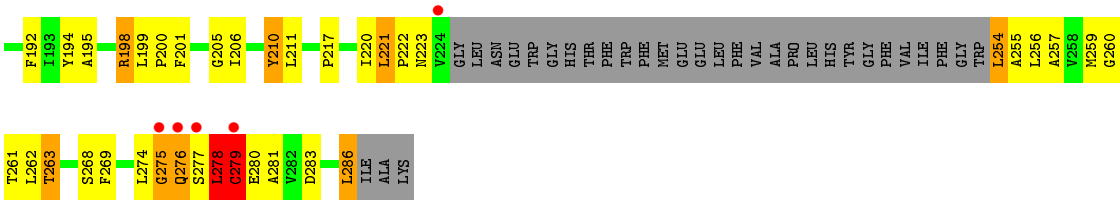
Position	Amino Acid	Information Content (bits)
1	GLY	0.00
2	THR	0.00
3	PRO	0.00
4	GLU	0.00
5	TYR	0.00
6	ILE	0.00
7	ARG	0.00
8	MET	0.00
9	VAL	0.00
10	GLU	0.00
11	LYS	0.00
12	GLY	0.00
13	THR	0.00
14	LEU	0.00
15	ARG	0.00
16	THR	0.00
17	PHE	0.00
18	GLY	0.00
19	LYS	0.00
20	ASP	0.00
21	VAL	0.00
22	A213	0.00
23	P214	0.00
24	F219	0.00
25	M223	0.00
26	F233	0.00
27	R236	0.00
28	W237	0.00
29	F238	0.00
30	S239	0.00
31	M240	0.00
32	L244	0.00
33	Q245	0.00
34	SER	0.00
35	THR	0.00
36	G95	0.00
37	E100	0.00
38	W101	0.00
39	R104	0.00
40	M107	0.00
41	F108	0.00
42	R111	0.00
43	T112	0.00
44	I116	0.00
45	M117	0.00
46	F118	0.00
47	V119	0.00
48	I129	0.00
49	D132	0.00
50	L136	0.00
51	M136	0.00
52	L137	0.00
53	S138	0.00
54	L142	0.00
55	I146	0.00
56	M150	0.00
57	G151	0.00
58	W152	0.00
59	Y157	0.00
60	W161	0.00
61	P162	0.00
62	I163	0.00
63	T164	0.00
64	A165	0.00
65	P166	0.00
66	V169	0.00
67	P170	0.00
68	W171	0.00
69	E172	0.00
70	M176	0.00
71	L177	0.00
72	I180	0.00
73	A181	0.00
74	Q184	0.00
75	G185	0.00
76	R190	0.00
77	Q95	0.00
78	E100	0.00
79	W101	0.00
80	R104	0.00
81	M107	0.00
82	F108	0.00
83	R111	0.00
84	T112	0.00
85	I116	0.00
86	M117	0.00
87	F118	0.00
88	V119	0.00
89	I129	0.00
90	D132	0.00
91	L136	0.00
92	M136	0.00
93	L137	0.00
94	S138	0.00
95	L142	0.00
96	I146	0.00
97	M150	0.00
98	G151	0.00
99	W152	0.00
100	Y157	0.00
101	W161	0.00
102	P162	0.00
103	I163	0.00
104	T164	0.00
105	A165	0.00
106	P166	0.00
107	V169	0.00
108	P170	0.00
109	W171	0.00
110	E172	0.00
111	M176	0.00
112	L177	0.00
113	I180	0.00
114	A181	0.00
115	Q184	0.00
116	G185	0.00
117	R190	0.00
118	Q95	0.00
119	E100	0.00
120	W101	0.00
121	R104	0.00
122	M107	0.00
123	F108	0.00
124	R111	0.00
125	T112	0.00
126	I116	0.00
127	M117	0.00
128	F118	0.00
129	V119	0.00
130	I129	0.00
131	D132	0.00
132	L136	0.00
133	M136	0.00
134	L137	0.00
135	S138	0.00
136	L142	0.00
137	I146	0.00
138	M150	0.00
139		

Chain F:

Met	Ser	Ala	Glu	Ser	A7	V8	S10	H11	T20	I21	D22	W23	M24	V28	V29	F30	V34	Y37	H38	I39	H40	A41	M42	M45	G46	D47	M48	W54	K55	W60	V61	T62	V63	T64	P65	I66	V69	T70	F71	P72	V75	Q76	S77	Y78	L79	Y83	P84
Met	Ser	Ala	Glu	Ser	A7	V8	S10	H11	T20	I21	D22	W23	M24	V28	V29	F30	V34	Y37	H38	I39	H40	A41	M42	M45	G46	D47	M48	W54	K55	W60	V61	T62	V63	T64	P65	I66	V69	T70	F71	P72	V75	Q76	S77	Y78	L79	Y83	P84







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 <sub>2</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.14Å 264.14Å 150.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.46 – 2.80 29.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.46-2.80) 91.2 (29.46-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.269 , 0.296 0.266 , 0.292	Depositor DCC
$R_{free}$ test set	5932 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 31.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 118193 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	19737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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

### 5.1 Standard geometry

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	0.83	2/3099 (0.1%)	0.87	3/4215 (0.1%)
1	E	0.81	2/3099 (0.1%)	0.87	5/4215 (0.1%)
1	I	0.74	1/3099 (0.0%)	0.79	2/4215 (0.0%)
2	B	0.75	0/1868	0.78	4/2560 (0.2%)
2	F	0.69	0/1868	0.75	3/2560 (0.1%)
2	J	0.70	0/1868	0.74	1/2560 (0.0%)
3	C	0.68	0/1822	0.75	1/2495 (0.0%)
3	G	0.62	0/1822	0.72	1/2495 (0.0%)
3	K	0.62	0/1822	0.71	1/2495 (0.0%)
All	All	0.73	5/20367 (0.0%)	0.79	21/27810 (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	2
1	E	0	2
1	I	0	3
2	B	0	1
2	F	0	1
2	J	0	2
3	C	0	2
3	K	0	2
All	All	0	15

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	288	ASP	CB-CG	5.98	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	ASP	CB-CG	5.94	1.64	1.51
1	E	338	GLU	CG-CD	5.32	1.59	1.51
1	I	288	ASP	CB-CG	5.07	1.62	1.51
1	A	343	GLU	CG-CD	5.01	1.59	1.51

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	326	ASP	CB-CG-OD1	11.33	128.49	118.30
1	E	326	ASP	CB-CG-OD2	-9.13	110.09	118.30
1	A	79	GLU	C-N-CA	6.32	137.51	121.70
2	B	47	ASP	N-CA-C	6.32	128.07	111.00
1	A	80	THR	N-CA-CB	5.95	121.60	110.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	VAL	Peptide
1	A	79	GLU	Peptide
2	B	46	GLY	Peptide
3	C	275	GLY	Peptide
3	C	277	SER	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	3017	0	2980	121	0
1	E	3017	0	2980	96	0
1	I	3017	0	2980	102	0
2	B	1796	0	1751	68	0
2	F	1796	0	1751	63	0
2	J	1796	0	1751	66	0
3	C	1759	0	1717	81	0
3	G	1759	0	1717	63	0
3	K	1759	0	1717	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
6	A	2	0	0	0	0
6	E	2	0	0	0	0
6	I	2	0	0	0	0
7	C	1	0	0	0	0
7	G	1	0	0	0	0
7	K	1	0	0	0	0
All	All	19737	0	19344	629	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 16.

The worst 5 of 629 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:C:275:GLY:HA2	3:C:276:GLN:CB	1.67	1.25
3:C:275:GLY:CA	3:C:276:GLN:HB2	1.66	1.22
3:K:275:GLY:HA2	3:K:276:GLN:CB	1.71	1.19
3:K:275:GLY:CA	3:K:276:GLN:HB2	1.72	1.16
3:G:275:GLY:HA2	3:G:276:GLN:CB	1.76	1.15

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	380/414 (92%)	336 (88%)	38 (10%)	6 (2%)	12	38
1	E	380/414 (92%)	347 (91%)	26 (7%)	7 (2%)	11	34
1	I	380/414 (92%)	340 (90%)	34 (9%)	6 (2%)	12	38
2	B	214/247 (87%)	189 (88%)	19 (9%)	6 (3%)	6	21
2	F	214/247 (87%)	185 (86%)	22 (10%)	7 (3%)	5	16
2	J	214/247 (87%)	187 (87%)	20 (9%)	7 (3%)	5	16
3	C	209/289 (72%)	168 (80%)	27 (13%)	14 (7%)	1	4
3	G	209/289 (72%)	165 (79%)	33 (16%)	11 (5%)	2	7
3	K	209/289 (72%)	168 (80%)	28 (13%)	13 (6%)	2	5
All	All	2409/2850 (84%)	2085 (87%)	247 (10%)	77 (3%)	5	17

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	A	225	ASP
1	A	288	ASP
2	B	45	MET
3	C	46	LEU

### 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	323/345 (94%)	294 (91%)	29 (9%)	12	34
1	E	323/345 (94%)	292 (90%)	31 (10%)	10	29
1	I	323/345 (94%)	296 (92%)	27 (8%)	14	37
2	B	186/210 (89%)	172 (92%)	14 (8%)	17	43
2	F	186/210 (89%)	168 (90%)	18 (10%)	10	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	186/210 (89%)	172 (92%)	14 (8%)	17	43
3	C	180/237 (76%)	162 (90%)	18 (10%)	9	27
3	G	180/237 (76%)	159 (88%)	21 (12%)	7	20
3	K	180/237 (76%)	161 (89%)	19 (11%)	8	24
All	All	2067/2376 (87%)	1876 (91%)	191 (9%)	11	32

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	360	ARG
1	I	277	LEU
3	G	117	ARG
1	E	385	SER
1	I	140	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	306	ASN
1	I	62	ASN
3	K	91	ASN
1	E	401	GLN
1	I	143	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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	$\# Z  > 2$
6	CUA	A	416	1	0,1,1	0.00	-	0,0,0	0.00	-
6	CUA	E	416	1	0,1,1	0.00	-	0,0,0	0.00	-
6	CUA	I	416	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
6	CUA	A	416	1	-	0/0/0/0	0/0/0/0
6	CUA	E	416	1	-	0/0/0/0	0/0/0/0
6	CUA	I	416	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

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 [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	382/414 (92%)	-0.49	5 (1%) 79 71	36, 56, 86, 109	0
1	E	382/414 (92%)	-0.43	7 (1%) 71 61	34, 57, 107, 129	0
1	I	382/414 (92%)	-0.44	6 (1%) 74 66	40, 63, 101, 126	0
2	B	218/247 (88%)	-0.10	3 (1%) 78 69	43, 64, 91, 106	0
2	F	218/247 (88%)	-0.06	6 (2%) 56 44	40, 70, 110, 144	0
2	J	218/247 (88%)	-0.16	4 (1%) 71 61	40, 71, 109, 137	0
3	C	213/289 (73%)	0.01	10 (4%) 35 24	59, 87, 122, 130	0
3	G	213/289 (73%)	0.17	15 (7%) 19 11	75, 100, 146, 155	0
3	K	213/289 (73%)	0.18	20 (9%) 11 5	70, 96, 147, 171	0
All	All	2439/2850 (85%)	-0.21	76 (3%) 52 40	34, 68, 121, 171	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	81	PHE	5.0
3	G	81	PHE	4.9
1	E	221	ALA	4.8
3	C	87	THR	4.7
1	I	231	THR	4.6

### 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
4	CU	I	415	1/1	0.99	0.03	-1.68	51,51,51,51	0
6	CUA	I	416	2/2	0.98	0.08	-1.69	74,74,74,85	0
6	CUA	A	416	2/2	0.96	0.08	-1.70	76,76,76,91	0
4	CU	E	415	1/1	0.99	0.05	-2.02	58,58,58,58	0
4	CU	A	415	1/1	0.99	0.03	-3.21	58,58,58,58	0
6	CUA	E	416	2/2	0.97	0.06	-4.73	59,59,59,79	0
5	ZN	A	800	1/1	0.98	0.03	-	74,74,74,74	0
5	ZN	K	663	1/1	0.99	0.02	-	66,66,66,66	0
5	ZN	F	664	1/1	0.91	0.19	-	139,139,139,139	1
5	ZN	E	800	1/1	0.41	0.57	-	146,146,146,146	0
5	ZN	J	664	1/1	0.87	0.23	-	145,145,145,145	1
5	ZN	I	800	1/1	0.68	0.41	-	158,158,158,158	0
5	ZN	G	663	1/1	0.98	0.08	-	65,65,65,65	0
5	ZN	C	663	1/1	0.99	0.04	-	56,56,56,56	0
5	ZN	B	664	1/1	0.98	0.09	-	48,48,48,48	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.