



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:54 AM GMT

PDB ID : 3CHX
Title : Crystal structure of Methylosinus trichosporium OB3b particulate methane monooxygenase (pMMO)
Authors : Hakemian, A.S.
Deposited on : 2008-03-10
Resolution : 3.90 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

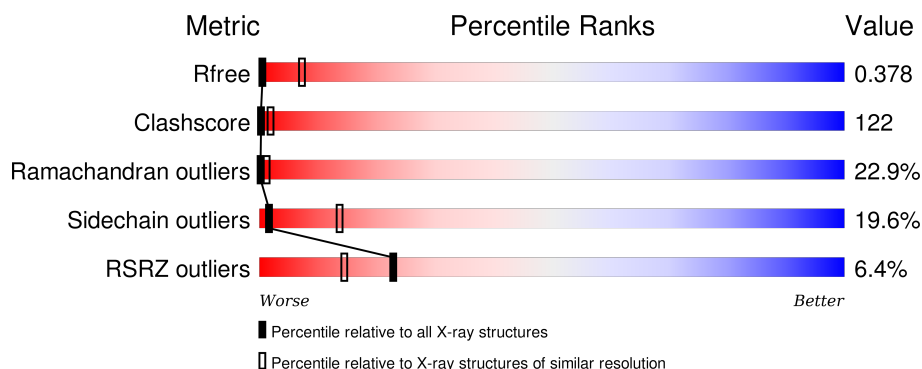
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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 ≥ 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	392	<div> <div>6%</div> <div>10%</div> <div>59%</div> <div>21%</div> <div>•</div> <div>8%</div> </div>
1	E	392	<div> <div>4%</div> <div>10%</div> <div>58%</div> <div>22%</div> <div>•</div> <div>8%</div> </div>
1	I	392	<div> <div>8%</div> <div>11%</div> <div>58%</div> <div>21%</div> <div>•</div> <div>8%</div> </div>
2	B	252	<div> <div>5%</div> <div>6%</div> <div>46%</div> <div>32%</div> <div>10%</div> <div>6%</div> </div>
2	F	252	<div> <div>5%</div> <div>7%</div> <div>46%</div> <div>32%</div> <div>10%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	252	<div><div></div><div>7%7%46%32%10%6%</div></div>
3	C	256	<div><div></div><div>3%6%36%18%38%</div></div>
3	G	256	<div><div></div><div>4%6%36%18%38%</div></div>
3	K	256	<div><div></div><div>6%7%36%18%38%</div></div>
4	D	20	<div><div></div><div>40%60%</div></div>
4	H	20	<div><div></div><div>40%60%</div></div>
4	L	20	<div><div></div><div>40%60%</div></div>
5	M	26	<div><div></div><div>19%81%</div></div>
5	N	26	<div><div></div><div>19%81%</div></div>
5	O	26	<div><div></div><div>19%81%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18945 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
1	A	362	Total	C	N	O	S	0	0	0
			2832	1831	478	518	5			
1	E	362	Total	C	N	O	S	0	0	0
			2832	1831	478	518	5			
1	I	362	Total	C	N	O	S	0	0	0
			2832	1831	478	518	5			

- Molecule 2 is a protein called PmoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1925	1303	301	310	11			
2	F	238	Total	C	N	O	S	0	0	0
			1925	1303	301	310	11			
2	J	238	Total	C	N	O	S	0	0	0
			1925	1303	301	310	11			

- Molecule 3 is a protein called PmoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	159	Total	C	N	O	S	0	0	0
			1324	886	211	223	4			
3	G	159	Total	C	N	O	S	0	0	0
			1324	886	211	223	4			
3	K	159	Total	C	N	O	S	0	0	0
			1324	886	211	223	4			

- Molecule 4 is a protein called 20-residue peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	20	Total	C	N	O	0	0	0
			100	60	20	20			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	20	Total	C	N	O	0	0	0
			100	60	20	20			
4	L	20	Total	C	N	O	0	0	0
			100	60	20	20			

- Molecule 5 is a protein called 26-residue peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	26	Total	C	N	O	0	0	0
			131	78	26	27			
5	N	26	Total	C	N	O	0	0	0
			131	78	26	27			
5	O	26	Total	C	N	O	0	0	0
			131	78	26	27			

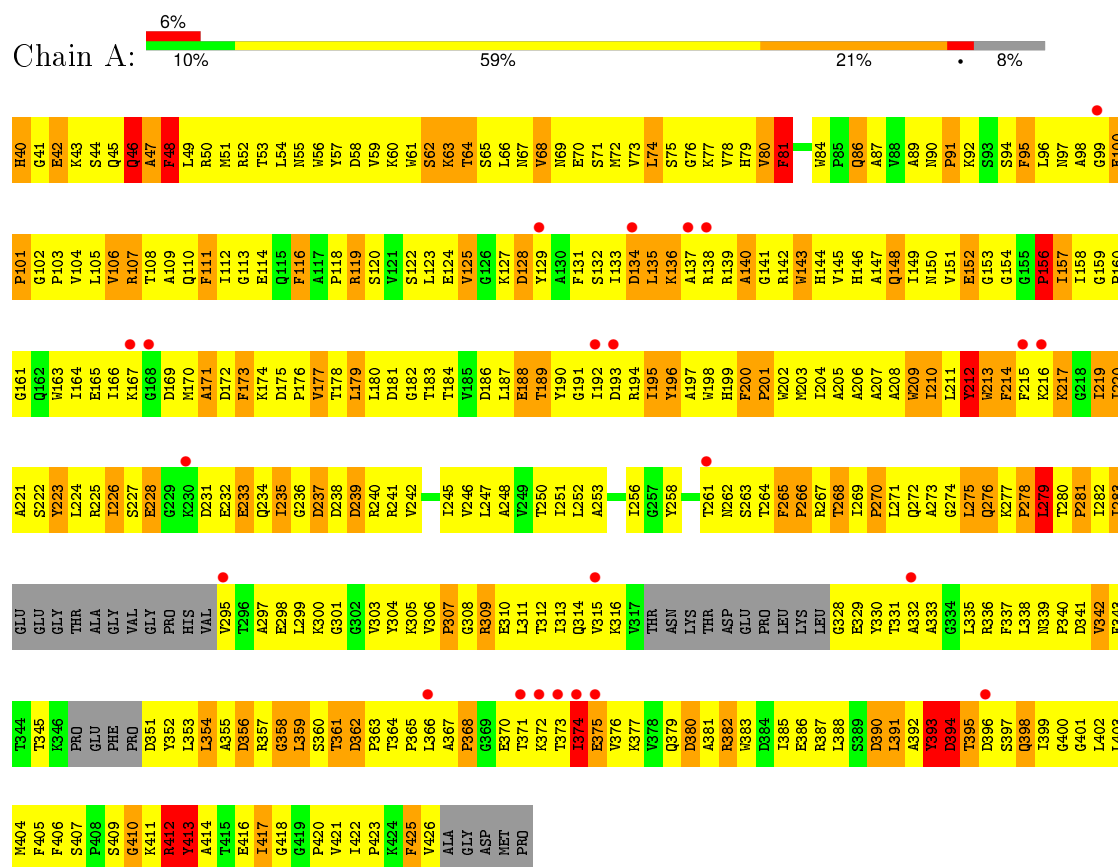
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

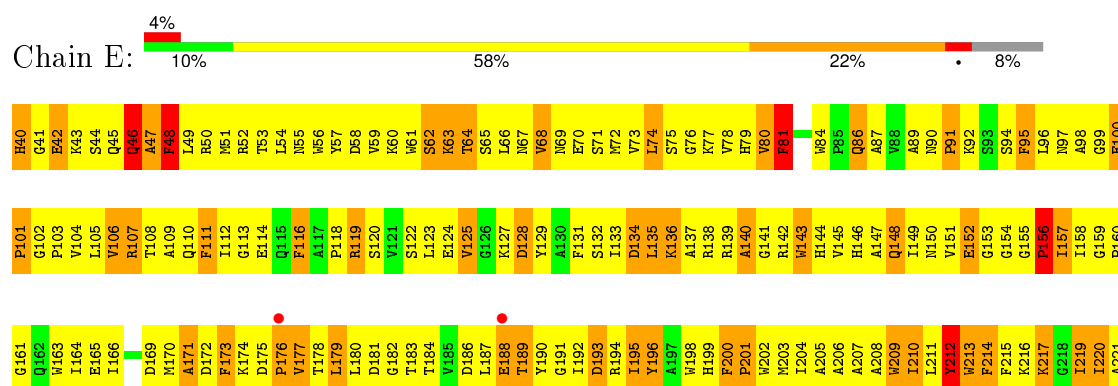
3 Residue-property plots

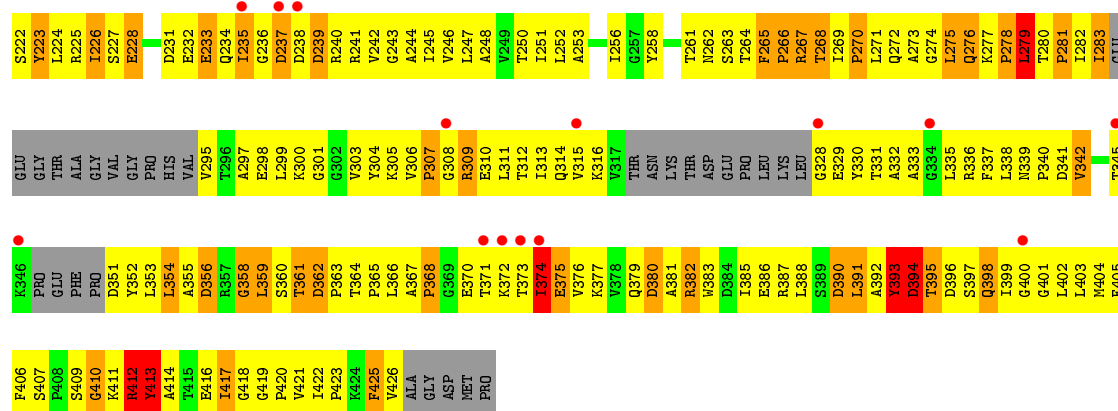
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PmoB

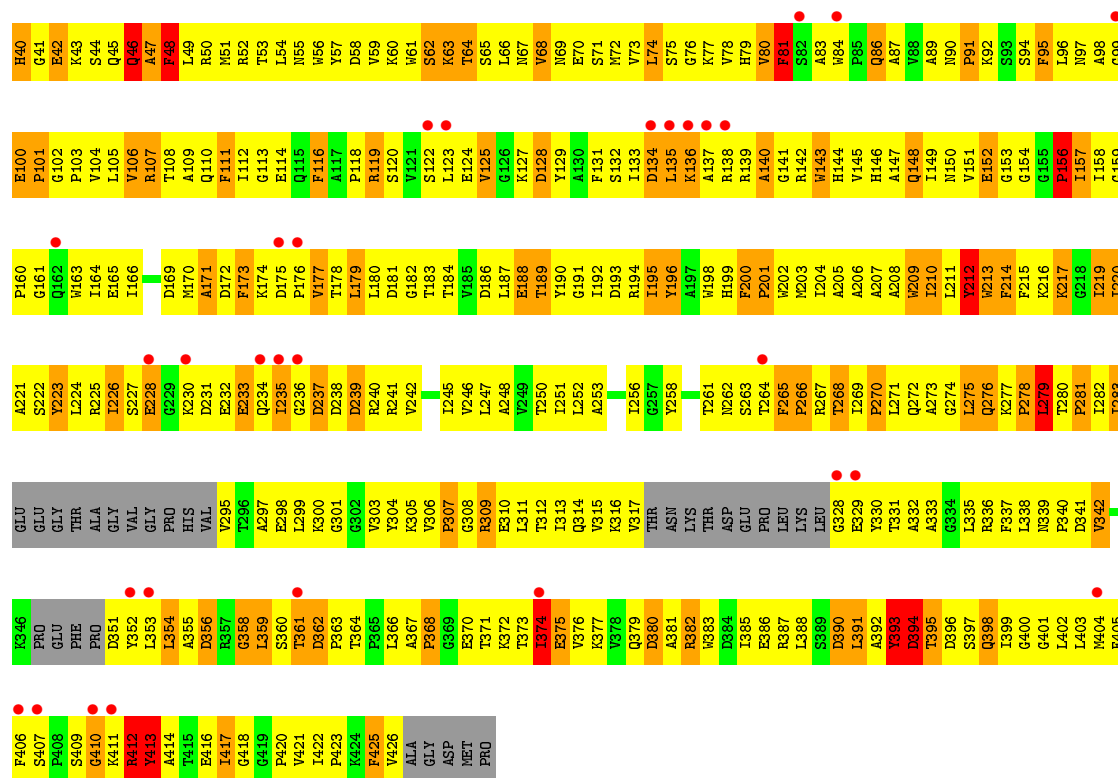
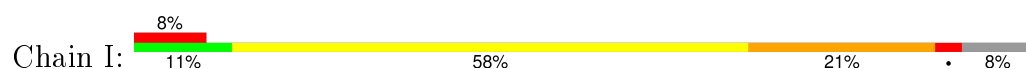


• Molecule 1: PmoB

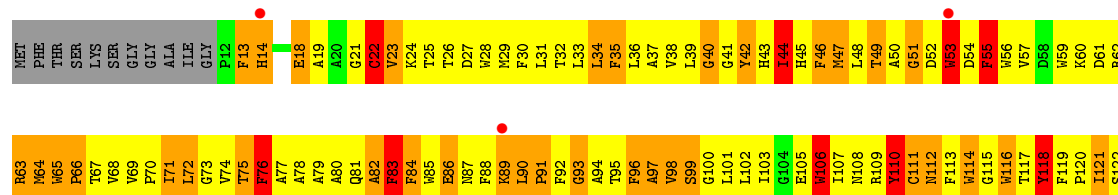


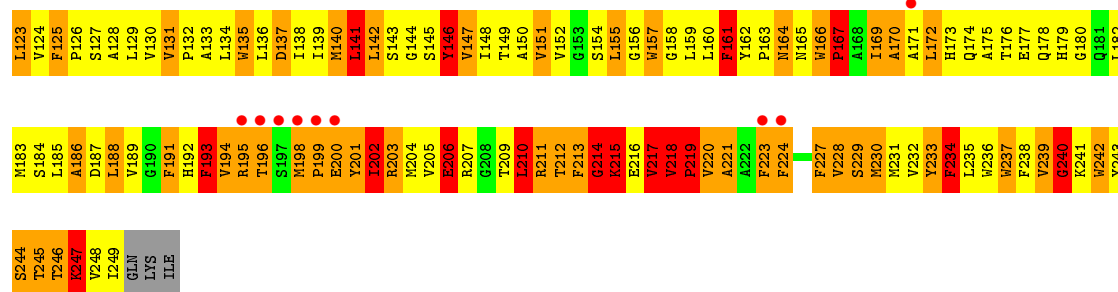


• Molecule 1: PmoB

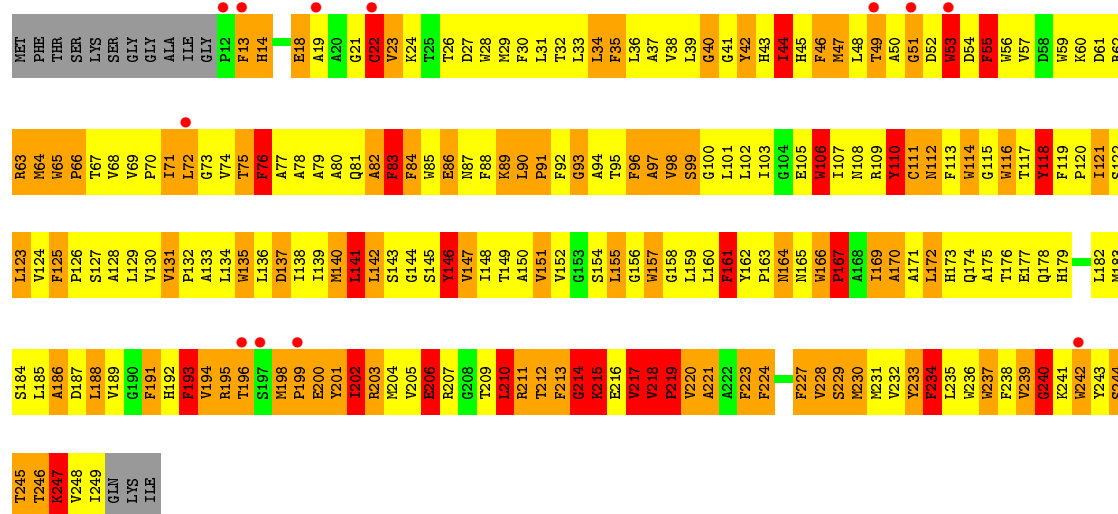


• Molecule 2: PmoA

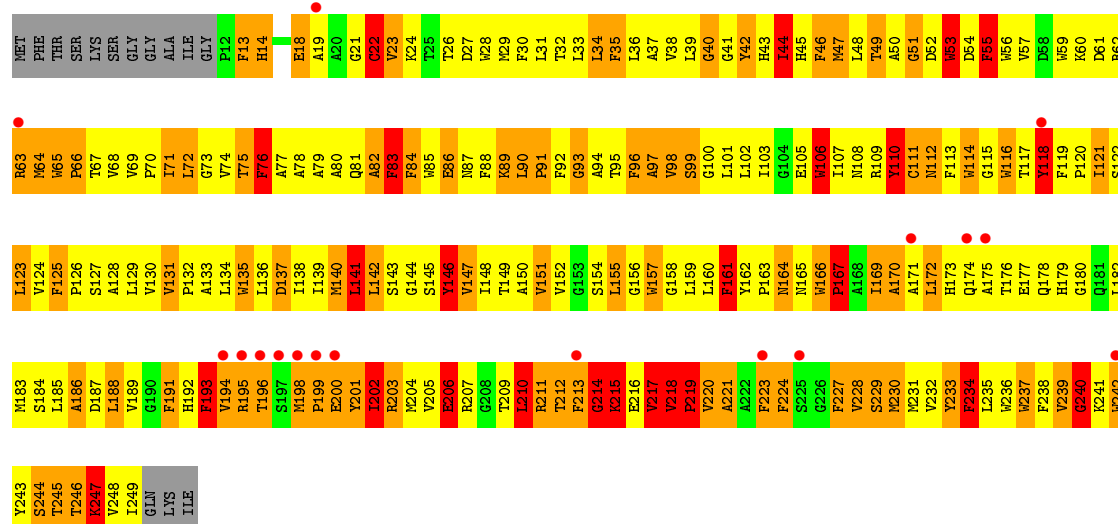




• Molecule 2: PmoA



• Molecule 2: PmoA

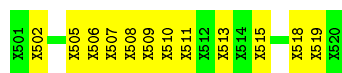


• Molecule 3: PmoC

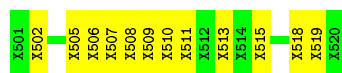


LYS
ARG
LEU
ILE
GLY
LYS
ASP
CYS
VAL
ALA
ALA
LEU
VAL
GLY

- Chain D: 40% 60%



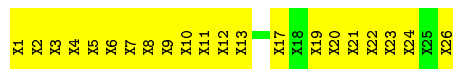
- Chain H: 40% 60%



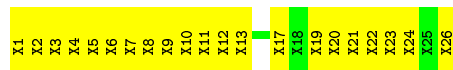
- Chain L:  40% 60%



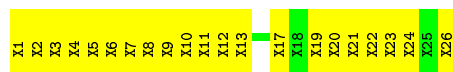
- Chain M: 19% 81%



- Chain N:  19% 81%



- Chain O: 19% 81%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.81Å 184.07Å 203.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 3.90 37.97 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.00-3.90) 99.9 (37.97-3.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 3.87Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.342 , 0.377 0.351 , 0.378	Depositor DCC
R_{free} test set	3992 reflections (10.06%)	DCC
Wilson B-factor (Å ²)	121.3	Xtriage
Anisotropy	0.991	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 102.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 39694 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	18945	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.48	0/2902	0.82	4/3944 (0.1%)
1	E	0.49	0/2902	0.82	4/3944 (0.1%)
1	I	0.48	0/2902	0.82	3/3944 (0.1%)
2	B	0.57	0/2002	0.88	7/2740 (0.3%)
2	F	0.57	0/2002	0.88	7/2740 (0.3%)
2	J	0.57	0/2002	0.88	7/2740 (0.3%)
3	C	0.50	0/1371	0.75	0/1876
3	G	0.50	0/1371	0.75	0/1876
3	K	0.50	0/1371	0.75	0/1876
All	All	0.52	0/18825	0.83	32/25680 (0.1%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	53	TRP	N-CA-C	-7.74	90.10	111.00
2	B	53	TRP	N-CA-C	-7.72	90.14	111.00
2	F	53	TRP	N-CA-C	-7.71	90.19	111.00
1	I	362	ASP	N-CA-C	-6.98	92.16	111.00
1	A	362	ASP	N-CA-C	-6.97	92.17	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2832	0	2837	705	1
1	E	2832	0	2837	707	0
1	I	2832	0	2837	709	1
2	B	1925	0	1884	600	0
2	F	1925	0	1884	609	0
2	J	1925	0	1884	603	0
3	C	1324	0	1292	324	0
3	G	1324	0	1292	328	0
3	K	1324	0	1292	322	0
4	D	100	0	22	17	0
4	H	100	0	22	17	0
4	L	100	0	22	18	0
5	M	131	0	28	30	0
5	N	131	0	28	30	0
5	O	131	0	28	30	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
6	E	2	0	0	0	0
6	G	1	0	0	0	0
6	I	2	0	0	0	0
6	K	1	0	0	0	0
All	All	18945	0	18189	4515	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 122.

The worst 5 of 4515 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:E:114:GLU:HG3	1:E:280:THR:HB	1.25	1.19
1:E:309:ARG:HD2	1:E:381:ALA:HA	1.22	1.16
1:I:359:LEU:HD21	1:I:376:VAL:HG13	1.17	1.15
1:A:359:LEU:HD21	1:A:376:VAL:HG13	1.17	1.15
1:A:309:ARG:HD2	1:A:381:ALA:HA	1.22	1.14

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)
1:A:167:LYS:NZ	1:I:230:LYS:NZ[3_555]	1.64	0.56

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	354/392 (90%)	206 (58%)	86 (24%)	62 (18%)	0	3
1	E	354/392 (90%)	206 (58%)	85 (24%)	63 (18%)	0	3
1	I	354/392 (90%)	206 (58%)	86 (24%)	62 (18%)	0	3
2	B	236/252 (94%)	87 (37%)	74 (31%)	75 (32%)	0	0
2	F	236/252 (94%)	87 (37%)	74 (31%)	75 (32%)	0	0
2	J	236/252 (94%)	87 (37%)	74 (31%)	75 (32%)	0	0
3	C	157/256 (61%)	72 (46%)	51 (32%)	34 (22%)	0	1
3	G	157/256 (61%)	72 (46%)	51 (32%)	34 (22%)	0	1
3	K	157/256 (61%)	72 (46%)	51 (32%)	34 (22%)	0	1
All	All	2241/2700 (83%)	1095 (49%)	632 (28%)	514 (23%)	0	1

5 of 514 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	48	PHE
1	A	68	VAL
1	A	81	PHE
1	A	140	ALA

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	298/322 (92%)	251 (84%)	47 (16%)	3	23
1	E	298/322 (92%)	250 (84%)	48 (16%)	3	22
1	I	298/322 (92%)	251 (84%)	47 (16%)	3	23
2	B	197/207 (95%)	143 (73%)	54 (27%)	0	5
2	F	197/207 (95%)	143 (73%)	54 (27%)	0	5
2	J	197/207 (95%)	143 (73%)	54 (27%)	0	5
3	C	135/208 (65%)	113 (84%)	22 (16%)	3	22
3	G	135/208 (65%)	113 (84%)	22 (16%)	3	22
3	K	135/208 (65%)	113 (84%)	22 (16%)	3	22
All	All	1890/2211 (86%)	1520 (80%)	370 (20%)	1	14

5 of 370 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	394	ASP
2	F	200	GLU
2	J	228	VAL
2	F	22	CYS
2	F	114	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	150	ASN
2	F	112	ASN
2	J	174	GLN
1	E	199	HIS
1	E	314	GLN

5.3.3 RNA ⓘ

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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

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, 95th 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 ²)	Q<0.9
1	A	362/392 (92%)	0.29	23 (6%) 23 14	145, 145, 145, 145	0
1	E	362/392 (92%)	0.16	16 (4%) 38 27	145, 145, 145, 145	0
1	I	362/392 (92%)	0.40	30 (8%) 14 9	145, 145, 145, 145	0
2	B	238/252 (94%)	0.10	12 (5%) 32 24	145, 145, 145, 145	0
2	F	238/252 (94%)	0.12	12 (5%) 32 24	145, 145, 145, 145	0
2	J	238/252 (94%)	0.17	17 (7%) 19 12	145, 145, 145, 145	0
3	C	159/256 (62%)	0.31	8 (5%) 32 24	145, 145, 145, 145	0
3	G	159/256 (62%)	0.24	11 (6%) 20 13	145, 145, 145, 145	0
3	K	159/256 (62%)	0.32	16 (10%) 9 7	145, 145, 145, 145	0
4	D	0/20	-	-	-	-
4	H	0/20	-	-	-	-
4	L	0/20	-	-	-	-
5	M	0/26	-	-	-	-
5	N	0/26	-	-	-	-
5	O	0/26	-	-	-	-
All	All	2277/2838 (80%)	0.24	145 (6%) 23 14	145, 145, 145, 145	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	THR	6.9
2	J	199	PRO	6.8
2	B	199	PRO	6.8
3	G	139	ASP	6.1
3	C	139	ASP	5.7

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, 95th 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(\AA^2)	Q<0.9
6	CU	G	662	1/1	0.97	0.35	-0.13	118,118,118,118	0
6	CU	A	711	1/1	0.99	0.19	-0.87	119,119,119,119	0
6	CU	I	731	1/1	0.94	0.15	-1.03	119,119,119,119	0
6	CU	K	663	1/1	0.92	0.16	-1.19	118,118,118,118	0
6	CU	C	661	1/1	0.89	0.17	-1.47	118,118,118,118	0
6	CU	E	721	1/1	0.94	0.09	-2.63	119,119,119,119	0
6	CU	E	722	1/1	0.90	0.22	-	127,127,127,127	0
6	CU	I	732	1/1	0.94	0.26	-	127,127,127,127	0
6	CU	A	712	1/1	0.97	0.17	-	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.