



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3BP8 / pdb_00003bp8
Title : Crystal structure of Mlc/EIIB complex
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Deposited on : 2007-12-18
Resolution : 2.85 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

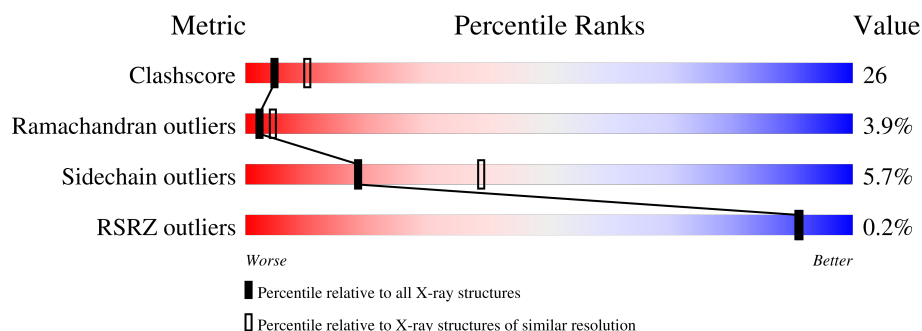
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	
2	C	75	
2	D	75	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6943 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative NAGC-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	71	0	0
			2927	1849	514	552	12			
1	B	380	Total	C	N	O	S	160	0	0
			2918	1846	512	547	13			

- Molecule 2 is a protein called PTS system glucose-specific EIICB component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	S	30	0	0
			542	338	95	106	3			
2	D	75	Total	C	N	O	S	34	0	0
			542	338	95	106	3			

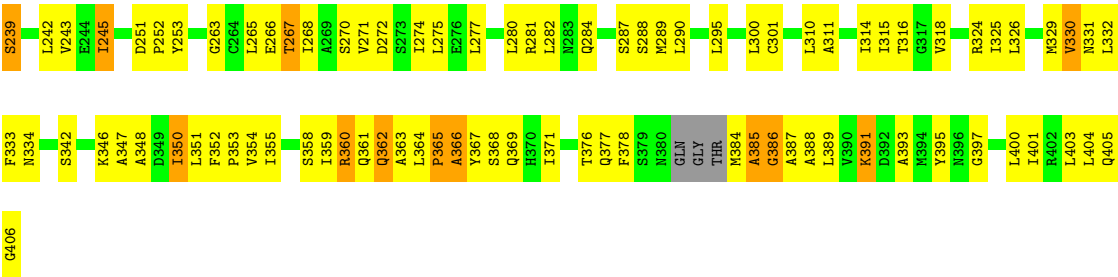
- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

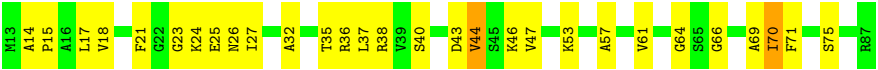
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0



● Molecule 2: PTS system glucose-specific EIICB component



● Molecule 2: PTS system glucose-specific EIICB component



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.43Å 55.42Å 82.46Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 20.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	83.2 (20.00-2.85) 92.0 (20.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.301 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6943	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, ACT

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	0.63	0/2972	1.09	17/4026 (0.4%)
1	B	0.58	0/2963	1.01	14/4013 (0.3%)
2	C	0.68	0/545	0.98	0/732
2	D	0.53	0/545	0.95	1/732 (0.1%)
All	All	0.61	0/7025	1.04	32/9503 (0.3%)

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(°)
1	A	240	SER	N-CA-C	-13.58	97.18	113.88
1	A	105	SER	N-CA-C	-8.87	102.47	113.38
1	A	13	ILE	N-CA-C	-8.40	103.59	113.42
1	A	159	THR	N-CA-C	7.06	119.83	111.71
1	A	282	LEU	N-CA-C	-6.58	105.55	113.97

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	2927	0	2976	150	0
1	B	2918	0	2978	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	542	0	563	27	0
2	D	542	0	563	28	0
3	A	12	0	9	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	6943	0	7089	341	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 26.

The worst 5 of 341 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:A:53:GLU:HB3	1:A:404:LEU:HD21	1.38	1.03
1:B:193:GLN:HB2	1:B:389:LEU:HD21	1.53	0.91
1:A:100:ALA:HB2	1:A:111:GLU:HG3	1.51	0.90
1:B:267:THR:HG22	1:B:268:ILE:HD12	1.52	0.90
1:B:157:ILE:HG21	1:B:192:ILE:HG21	1.58	0.83

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	375/406 (92%)	313 (84%)	45 (12%)	17 (4%)	2	3
1	B	374/406 (92%)	310 (83%)	50 (13%)	14 (4%)	2	5
2	C	73/75 (97%)	62 (85%)	9 (12%)	2 (3%)	4	9
2	D	73/75 (97%)	63 (86%)	8 (11%)	2 (3%)	4	9
All	All	895/962 (93%)	748 (84%)	112 (12%)	35 (4%)	2	4

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ALA
1	A	249	GLN
1	A	280	LEU
1	B	26	ASP
1	B	123	PRO

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	320/339 (94%)	305 (95%)	15 (5%)	23	47
1	B	320/339 (94%)	296 (92%)	24 (8%)	12	26
2	C	56/56 (100%)	53 (95%)	3 (5%)	20	42
2	D	56/56 (100%)	55 (98%)	1 (2%)	51	73
All	All	752/790 (95%)	709 (94%)	43 (6%)	18	39

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	267	THR
1	B	369	GLN
1	B	272	ASP
1	B	351	LEU
1	B	378	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	139	HIS
1	B	223	ASN
1	B	217	GLN
1	B	405	GLN
1	A	334	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 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	$\# Z > 2$
3	ACT	A	408	-	3,3,3	0.87	0	3,3,3	0.52	0
3	ACT	A	409	-	3,3,3	0.92	0	3,3,3	0.58	0
3	ACT	A	407	-	3,3,3	0.88	0	3,3,3	0.64	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, 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	381/406 (93%)	-0.22	1 (0%) 90 89	12, 37, 60, 74	19 (4%)
1	B	380/406 (93%)	-0.03	1 (0%) 90 89	15, 43, 80, 93	42 (11%)
2	C	75/75 (100%)	-0.36	0 100 100	13, 34, 42, 53	7 (9%)
2	D	75/75 (100%)	0.16	0 100 100	23, 55, 78, 87	8 (10%)
All	All	911/962 (94%)	-0.12	2 (0%) 91 91	12, 40, 71, 93	76 (8%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	MET	2.5
1	B	46	SER	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	A	407	4/4	0.64	0.15	70,70,70,71	0
3	ACT	A	408	4/4	0.66	0.23	86,86,87,88	0
3	ACT	A	409	4/4	0.72	0.19	67,68,68,68	0
4	ZN	A	410	1/1	0.96	0.07	59,59,59,59	0
4	ZN	B	407	1/1	0.97	0.06	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.